Schrödinger difference equation with deterministic ergodic potentials

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Abstract

We review the recent developments in the theory of the one-dimensional tight-binding Schrödinger equation for a class of deterministic ergodic potentials. In the typical examples the potentials are generated by substitutional sequences, like the Fibonacci or the Thue-Morse sequence. We concentrate on rigorous results which will be explained rather than proved. The necessary mathematical background is provided in the text.

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1   Introduction

The one-dimensional Schrödinger equation

$$(-d^2/dx^2 + V(x))\psi(x) = E\psi(x)$$

has long been serving as a laboratory for studying a large variety of problems in Quantum Mechanics. Most often it appears as the eigenvalue equation of a one-electron energy operator, and then $V(x)$ means the potential energy of the electron. In Atomic or Molecular Physics $V(x)$ is typically fast-decaying or vanishes outside a bounded set, while in applications to Solid State Physics it is an extended function. Our concern will be the Schrödinger equation of Solid State Physics in the tight-binding approximation: the real axis is replaced by $\mathbf{Z}$, the lattice of integers, and the differential operator by the second order difference operator. The tight-binding Schrödinger equation describes an electron in a lattice in which the attraction of the ion cores slows down the interatomic motion of the electron: the kinetic energy has an *a priori* upper bound which does not exist in the continuous case.

The potentials we are going to consider are on the midway between periodic and random; in physics literature they are sometimes called 'aperiodic' or 'disordered deterministic'. They all fall into the family of the so-called strictly ergodic sequences. A typical subfamily which appeared regularly in the lectures of this Winter School are the substitutional sequences as, for example, the Fibonacci sequence. As we will see later, the periodic and the uniformly almost periodic sequences are also strictly ergodic, but a random potential is usually 'only' ergodic.

In this field physicists and mathematicians have been working parallelly during about the last fifteen years. The ambition of this course is to review and explain the contribution of the latter for an audience unfamiliar with the underlying mathematics. Most of the time, mathematicians consider the Schrödinger equation directly on the infinite chain $\mathbf{Z}$ or on the semi-infinite chain $\mathbf{N}$. The equation is then the 'eigenvalue equation' of an infinite matrix which is named after Jacobi. If the diagonal (the potential) is an ergodic sequence, the spectrum happens not to be a *discrete* point spectrum. It is rather often - at least within the family of potentials we are going to consider - singularly continuous and is, as an ensemble of points, a (generalized) Cantor set. These notions and many others, necessary for the understanding of the specific results will be introduced in the forthcoming sections.

We start, in Section 2, by the presentation of the main examples and the definition of strict ergodicity. The subject is developed in Sections 3, 4, 6 and 7. In Section 3 we give the basic ingredients of the theory of discrete Schrödinger equation in one dimension and introduce the notions of the transfer matrix and Lyapunov exponent. A subsection is devoted to the scattering problem and Landauer resistance. Section 4 contains some of the fundamental results for periodic potentials. Section 6 summarizes the general results obtained for one-dimensional Schrödinger operators with strictly ergodic potentials. Section 7 is a review of our actual knowledge about models with specific potentials, given by Sturmian and substitutional sequences.

Section 5 is an introduction into spectral theory. It is far more the longest part of the course, with the definitions of spectrum, essential spectrum, eigenvalue, point and continuous spectrum, spectral projections, measures and spectral measures, Cantor sets etc., illustrated with examples. Subordinacy and the classification of the spectrum according to the asymptotic behavior of the solutions of the Schrödinger equation is also discussed here.

The widely studied Almost-Mathieu or Harper equation is not presented in full detail but appears in examples throughout the whole text, and papers on it are included among the references.

Some more or less simple facts are announced in the form of problems. The reader may only retain the statements or, if he wishes, check his understanding by proving them. The solutions can be found in Section 8.

These notes are not written in a purely mathematical style. Proofs, unless they are really elementary, are replaced by explanations. This suffices for the physicist who wishes to understand the results but has no ambition to provide mathematical proofs of his own. The interested reader can find excellent monographs which present the subject with full mathematical rigor. Also, one should remember that nothing can replace the lecture of the original research papers. A rather detailed, although certainly incomplete, list of references is provided at the end of the notes. I thank François Monti for helping me to construct this list.

2   Main examples

The tight-binding Schrödinger equation in one dimension is written as

$$\psi_{n-1} + \psi_{n+1} + V_n \psi_n = E \psi_n \tag{2.1}$$

Here n runs over the integers, $V = \{V_n\}$ is a real sequence (the potential), E is a real number (the energy), although sometimes it is useful to take it complex. The problem is to find the 'physically allowed' values of E, that is, those admitting at least one 'not too fast increasing' solution, and to describe these solutions. The following potentials will be considered:

(1) $V_n = V(\omega)_n = \lambda \cos 2\pi(n\alpha + \omega)$, $\lambda \neq 0$. The corresponding discrete Schrödinger equation is called the Almost-Mathieu equation (because the continuous version is the Mathieu equation). The case $\lambda = 2$ is the Harper equation.

(2) $V_n = V(\omega)_n = \lambda X_A(n\alpha + \omega)$, where $\lambda \neq 0$, A is the union of semi-open intervals of $[0, 1)$ and $X_A(x) = 1$ if the fractional part of x falls into A and is zero otherwise. These are the so-called circle-potentials. An important special case is when A is a semi-open interval of length α: The $\{0, 1\}$-valued sequences

$$X_{[0,\alpha)}(n\alpha + \omega) = \lfloor n\alpha + \omega \rfloor - \lfloor (n-1)\alpha + \omega \rfloor$$
$$X_{(0,\alpha]}(n\alpha + \omega) = \lceil n\alpha + \omega \rceil - \lceil (n-1)\alpha + \omega \rceil \tag{2.2}$$

for irrational α are called Sturmian sequences. The notations $\lfloor \cdot \rfloor$ and $\lceil \cdot \rceil$ mean rounding downwards and upwards, respectively. If $\alpha = (\sqrt{5} - 1)/2$, we obtain the Fibonacci sequence. Generalized Fibonacci sequences (obtained through the substitution $\xi(a) = a^n b$ and $\xi(b) = a$ with $n \geq 1$) are also Sturmian. According to an equivalent definition, Sturmian sequences are the sequences with minimal complexity among the non-ultimately-periodic sequences (see e.g. [1], [23]).

(3) V is a substitutional sequence:

Let ξ be a primitive substitution ([114]) on a finite alphabet $\mathcal{A} = \{a_1, ..., a_r\}$, f a non-constant real function on $\mathcal{A}$. Suppose that $\xi(a) = ...a$ and $\xi(b) = b...$ for some $a, b \in \mathcal{A}$ and let $\omega = uv$ where u and v are the left- and right-sided fixed points of ξ: $u = \xi^\infty(a) = ...a$ and $v = \xi^\infty(b) = b....$ Then $V(\omega)_n = f(\omega_n)$. A comment on the concatenation uv will follow in Section 6. Generalized Fibonacci sequences have a natural definition on $\mathbf{Z}$ via the formula for Sturmian sequences.

The potentials defined in (1)-(3) are *strictly ergodic*, that is, *minimal* and *uniquely ergodic*:

(i) V is minimal.

Let T be the left shift, and denote $V(T\omega)$ the shifted potential: $V(T\omega)_n = V(\omega)_{n+1}$. The notation ($T$ applied to ω) may seem curious, however, in all cases $T\omega$ can be given a well-defined meaning. For potentials (1) and (2)

$$T\omega = \omega + \alpha \pmod 1$$

In case (3), $T\omega$ is the left-shifted sequence,

$$(T\omega)_n = \omega_{n+1}$$

The orbit of $V(\omega)$, i.e., the sequence of translates, $V(T^k\omega)$ for $k = ..., -1, 0, 1, ...$, has pointwise convergent subsequences: $W = \{W_n\}$ is called a pointwise limit of translates of $V(\omega)$ if for a suitably chosen sequence $\{k_i\}$, $V(T^{k_i}\omega)_n$ tends to W_n for every n. Clearly, $W = V(\omega')$, where ω' is the limit of $T^{k_i}\omega$ in cases (1) and (2) and is a pointwise limit of translates of ω in case (3).

The orbit of V together with all its pointwise limits is called the *hull* of V and is denoted by $\Omega(V)$. This is a kind of closure of the set of translates. The hull can be constructed for any infinite sequence. If V is periodic with period length L, the hull is a set of L elements. The potentials of (1) and (2) are periodic if α is rational. If α is irrational, the hull of $V = V(\omega = 0)$ is $\{V(\omega)\}_{\omega \in [0,1)}$! This is the typical situation: the hull is much larger (uncountable) than the set of translates (countable). If S is an arbitrary sequence and S' is a pointwise limit of translates of

S, the hull of S' is usually different from the hull of S. (Example: $S_n = 1 - 1/n, n = 1, 2, ...$ The translates have a single pointwise limit, $S'_n \equiv 1$. The only element of $\Omega(S')$ is S' itself.)

The potentials defined in (1)-(3) have the property that for any $W \in \Omega(V)$, $\Omega(W) = \Omega(V)$. This is what the minimality of V means. The V-independent hull is denoted by Ω. Clearly, every element of Ω is minimal and therefore the 'flow' (Ω, T) itself can be called minimal: every trajectory is dense in Ω (its closure is Ω) or equivalently, the only closed and shift-invariant subsets of Ω are the empty set and Ω.

Problem 1. (Cf. Queffélec [113]) Let $s = \{s_n\}_{-\infty}^{\infty}$ be a bounded complex sequence, $\Omega(s)$ its hull,

$$\Omega(s) = \overline{\{T^k s\}_{k=-\infty}^{\infty}}$$

where the bar means closure with respect to pointwise convergence. The following are equivalent.
1. s is minimal, i.e., for every $t \in \Omega(s)$, $\Omega(t) = \Omega(s)$.
2. For every $t \in \Omega(s)$, $s \in \Omega(t)$.
3. s is almost-periodic in the metric

$$d(s, t) = \sum_{n=-\infty}^{\infty} 2^{-|n|} |s_n - t_n|$$

i.e., for each $\varepsilon > 0$ there exists an $\ell_\varepsilon < \infty$ and a sequence $\{n_k\}_{k=-\infty}^{\infty}$ of integers with gaps bounded by ℓ_ε, $0 < n_{k+1} - n_k < \ell_\varepsilon$, such that for all k

$$d(T^{n_k} s, s) = \sum_{n=-\infty}^{\infty} 2^{-|n|} |s_{n+n_k} - s_n| \leq \varepsilon .$$

A sequence is called *recurrent* if it is the pointwise limit of its own translates. A minimal sequence is recurrent but a recurrent sequence may not be minimal. A counterexample is provided by the sequence of digits 1234567891011121314..., obtained by concatenating the positive integers, written, e.g., in base 10. It is the pointwise limit of its own left shifts, but is not minimal: words are repeated with increasing gaps. The hull of this sequence is the set of all sequences composed of the digits $0, 1, ..., 9$.

The different meanings, in different cases, of the label ω should not disturb the reader. In (1) and (2), ω is a number of the interval $[0, 1)$; in (3) it is an element of the hull of uv, and uv is also a minimal sequence.

(ii) V is uniquely ergodic.
Recall that the dynamical system (Ω, T, ρ), where ρ is a T-invariant probability measure, is ergodic if for any ρ-integrable function f

$$\lim_{N \to \infty} N^{-1} \sum_{n=1}^{N} f(T^n \omega_0) = \int_{\Omega} f(\omega) d\rho(\omega)$$

for ρ-almost every ω_0 (i.e., apart from a set of ω_0's of zero ρ-measure). Choosing f to be the characteristic function of a set A, it is seen that ergodicity implies that (in fact, is equivalent to) $\rho(A) = 0$ or 1 for every T-invariant set A.

The unique ergodicity of V means that there exists a unique shift-invariant probability measure ρ on $\Omega(V)$ ($\rho(T^{-1}A) = \rho(A)$ for any measurable $A \subset \Omega$).

Problem 2. If s is a uniquely ergodic sequence with shift-invariant probability measure ρ then $(\Omega(s), T, \rho)$ is ergodic.

In case (1) (Almost-Mathieu), the most natural way to obtain this measure is to define, for $0 \leq a < b < 1$,

$$\rho(A_{ab}) = b - a \quad , \quad \text{where } A_{ab} = \{V(\omega)\}_{a < \omega < b} \tag{2.3}$$

and to extend ρ to countable unions and intersections of the sets A_{ab} by using the properties of measures.

For substitutional potentials the usual construction is to assign probabilities to the so-called *cylinder sets* and to extend ρ to countable unions and intersections of cylinders. If $v = (v_1, v_2, ..., v_k)$

is a finite collection of real numbers and n is an integer, the cylinder $[v, n]$ is a family of potentials taken from the hull,

$$[v, n] = \{V \in \Omega : V_{n+i} = v_i, i = 1, \ldots, k\} \tag{2.4}$$

Noticing that the relative frequency of the 'word' v is the same in all $V \in \Omega$, the probability $\rho([v, n])$ can be defined as this relative frequency.

For circle potentials a shift-invariant ρ can be derived naturally either through Eq. (2.3) or through word frequencies. For the Almost-Mathieu potential cylinders can also be defined (by replacing, in Eq. (2.4), $V_{n+i} = v_i$ by $V_{n+i} \in I_i$, where I_i is an interval), and one can obtain a T-invariant probability measure through them. Uniqueness implies that the different constructions yield the same measurable sets and measures.

Physicists never worry (do not even have to know) about the hull; mathematicians all the time struggle with it. The reason is that in laboratory or computer experiments one deals with finite samples, and these may come from any element of the hull: therefore it is sufficient to keep just one. (However, the physicist's sample averaging is nothing else than averaging over the hull with the measure ρ.) The mathematician is naturally led to the notions of hull and strict ergodicity by working on the infinite system. He (she) has to consider V as a ρ-distributed random variable on Ω. The results she (he) obtains are valid either for a given $V \in \Omega$ or for every $V \in \Omega$ or, most often, for ρ-a.e. (almost every) $V \in \Omega$, i.e., $\rho(\{V \in \Omega$: the result is not valid$\}) = 0$. Notice that the distinction between 'every' and 'almost every' is by no means harmless. Indeed, because ρ is a continuous probability measure (that is, $\rho(\{V\}) = 0$ for every one-point subset of Ω), any countably infinite subset of the hull has zero probability. A surprising new result about an even larger (uncountable) set of vanishing ρ-measure, for which a claim (localization) is not valid, will be quoted in Section 5.2.

Problem 3. If ρ is a shift-invariant probability measure on Ω and the trajectory of every point is infinite then ρ is continuous.

3 General results on the Schrödinger difference equation

3.1 Basic observations

The first two terms of Eq.(2.1) correspond to the action of the kinetic energy operator on the wave function, and any physicist would prefer to replace them by

$$-\psi_{n-1} - \psi_{n+1} + 2\psi_n$$

This is, however, a difference of no importance: Omitting $2\psi_n$ means shifting the zero of the energy by 2, and changing the sign of the first two entries in Eq.(2.1) amounts to a unitary transformation, thus leaving the spectrum of the energy operator unchanged. Therefore a global change of sign of V is also of no importance: we get the mirror image of the spectrum. This simple fact can be expressed in a more shocking form: If V gives rise to a localized state at energy E, $-V$ will give rise to a localized state at energy $-E$. Or still in another form: There can exist extended states at energies everywhere below the potential, $E < V_n$ for all n.

Without saying otherwise, we always consider the Schrödinger equation on the infinite lattice **Z**. Equation (2.1) is a homogeneous linear second order difference equation. As a consequence, for any (complex) E the solutions form a two-dimensional linear vector space:

- If ψ^1 and ψ^2 solve (2.1), then $\psi = c_1\psi^1 + c_2\psi^2$ solves it for any complex c_1 and c_2.

- There *exist* two linearly independent solutions ψ^1 and ψ^2.

Two nontrivial ($\neq 0$) solutions are linearly *dependent* if and only if they are constant multiples of each other. When saying that Eq.(2.1) has a unique solution of some property, we will understand 'unique linearly independent'.

Writing (2.1) for ψ^1 and ψ^2 (not necessarily linearly independent), multiplying the first equation by ψ_n^2 and the second one by ψ_n^1 and subtracting we find that

$$\psi_{n+1}^1\psi_n^2 - \psi_n^1\psi_{n+1}^2 = \psi_n^1\psi_{n-1}^2 - \psi_{n-1}^1\psi_n^2 = \cdots = \psi_1^1\psi_0^2 - \psi_0^1\psi_1^2$$

This constant is the Wronskian and will be denoted by $W[\psi^1, \psi^2]$. As a consequence,

- ψ^1 and ψ^2 are linearly independent solutions if and only if $W[\psi^1, \psi^2] \neq 0$.

- There can be *at most* one solution going to zero as $n \to \infty$. If ψ^1 is such a solution, then for any other (linearly independent) solution ψ

$$|\psi_n|^2 + |\psi_{n+1}|^2 \to \infty \text{ as } n \to \infty$$

The same conclusion holds for the limit $n \to -\infty$. As a consequence, there can be *at most* one solution decaying on both sides, and if such a solution exists, all the others blow up on both sides.

3.2   Transfer matrices

We may rewrite the Schrödinger equation in the redundant vectorial form

$$\Psi_n = \begin{pmatrix} E - V_n & -1 \\ 1 & 0 \end{pmatrix} \Psi_{n-1} \equiv T_n \Psi_{n-1}$$

where

$$\Psi_n = \begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} \tag{3.1}$$

By iterating,

$$\Psi_n = T_n T_{n-1} \cdots T_1 \Psi_0 \equiv T_{1 \to n} \Psi_0$$

and similarly,

$$\Psi_{-n} = T_{-n+1}^{-1} T_{-n+2}^{-1} \cdots T_0^{-1} \Psi_0 = T_{0 \to -n+1} \Psi_0$$

The matrices T are called transfer matrices. Their determinant is 1: this is clear for T_n and its inverse and holds for the others because the determinant of a product of matrices is the product of the determinants.

The determinant of $T_{1 \to n}$ can be seen as the Wronskian of the two 'standard' solutions ψ^1 and ψ^2 with initial conditions

$$\begin{matrix} \psi_1^1 = 1 & 0 = \psi_1^2 \\ \psi_0^1 = 0 & 1 = \psi_0^2 \end{matrix}$$

In terms of these solutions the transfer matrix can be written as

$$T_{1 \to n} = T_{1 \to n} \begin{pmatrix} \psi_1^1 & \psi_1^2 \\ \psi_0^1 & \psi_0^2 \end{pmatrix} = \begin{pmatrix} \psi_{n+1}^1 & \psi_{n+1}^2 \\ \psi_n^1 & \psi_n^2 \end{pmatrix} \tag{3.2}$$

showing that indeed,

$$\det T_{1 \to n} = W[\psi^1, \psi^2] = 1$$

The general form of the transfer matrix from site m to site n is

$$T_{m \to n} = A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad, \quad ad - bc = 1 \tag{3.3}$$

Here a, b, c, d are polynomials of E with real coefficients and of degree $\leq |n - m| + 1$. In particular,

$$\text{tr } A = a + d = E^{|n-m|+1} + \cdots$$

For real energies the transfer matrices are elements of the group $\text{SL}(2,\mathbf{R})$. The characteristic equation of a matrix A in this group reads

$$\det(\lambda - A) = \lambda^2 - \lambda \text{ tr } A + 1 = 0$$

Therefore the two roots satisfy the relations $\lambda_1 \lambda_2 = 1$ and $\lambda_1 + \lambda_2 = \text{tr } A$. We can distinguish four cases:

1. The two roots are real, $|\lambda_1| = |\lambda_2^{-1}| > 1$, the corresponding eigenvectors are also real and nonorthogonal, in general. $|\operatorname{tr} A| > 2$, the matrix is *hyperbolic*.
   For example, the 'hyperbolic rotations'

$$\left(\begin{array}{cc} \cosh x & \sinh x \\ \sinh x & \cosh x \end{array} \right)$$

   are special (symmetric) hyperbolic matrices. $\lambda_{1,2} = \exp(\pm x)$, the corresponding eigenvectors are the transposed of $(1 \quad \pm 1)$.

2. $\lambda_1 = \lambda_2^* = e^{i\varphi}$, $\varphi \neq n\pi$. There are two complex eigenvectors. $\operatorname{tr} A = 2\cos\varphi$, the matrix is *elliptic*. As an example, the ordinary rotation matrix

$$\left(\begin{array}{cc} \cos x & -\sin x \\ \sin x & \cos x \end{array} \right)$$

   is elliptic. $\lambda_{1,2} = \exp(\pm ix)$, the eigenvectors are the transposed of $(1 \quad \mp i)$.

3. $\lambda_1 = \lambda_2 = \pm 1$. There is a unique, real, eigenvector (the geometric multiplicity is 1). $|\operatorname{tr} A| = 2$, the matrix is *parabolic*. An example is

$$\left(\begin{array}{cc} 1 & b \\ 0 & 1 \end{array} \right)$$

   with $b \neq 0$. The unique eigenvector is the transposed of $(1 \quad 0)$.

4. $A = \pm I$ where I is the unit matrix.

Some assertions will concern the norm of transfer matrices. The natural matrix norm

$$\|A\| = \sup \|Au\|/\|u\|$$

associated with the vector norm $\|u\| = (|u_1|^2 + |u_2|^2)^{\frac{1}{2}}$ satisfies

$$\|A\|^2 = \text{max. eigenvalue of } A^*A = \frac{1}{2}\|A\|_2^2 + \left(\frac{1}{4}\|A\|_2^4 - 1\right)^{\frac{1}{2}} = \|A^{-1}\|^2 \geq 1$$

$$(3.4)$$

Here $\|A\|_2$ is the trace norm,

$$\|A\|_2^2 = \operatorname{tr} A^*A = a^2 + b^2 + c^2 + d^2 = \|A^{-1}\|_2^2 \geq 2 \tag{3.5}$$

(cf. Eq.3.3), which proves also the last inequality in (3.4).

Let us return to the trace of the transfer matrix as a function of E.

$$\operatorname{tr} T_{1\to n}(E) = E^n + \cdots = p_n(E)$$

is an nth degree polynomial with n *distinct real* roots and the property that

$$\frac{\mathrm{d}}{\mathrm{d}E} p_n(E) \neq 0 \ \text{ if } \ |p_n(E)| < 2$$

In Figure 1a we represented the generic situation for $n = 5$: There are n disjoint intervals of the energy within which the transfer matrix is elliptic, separated by intervals of hyperbolicity. Figure 1b shows an atypical case for $n = 4$: Some intervals of hyperbolicity disappear because the derivative of the trace vanishes at the same E where the trace takes on the value 2 or -2.

   Problem 1. For $A \in \mathrm{SL}(2,\mathbf{R})$, show that $|\operatorname{tr} A^k| \leq 2$ if and only if $|\operatorname{tr} A| \leq 2$. Plot $\operatorname{tr} T_{1\to n}^3(E)$ on the top of Figure 1.

3.3 Lyapunov exponent

Consider

$$\gamma_n = \frac{1}{|n|} \ln \|T_{1 \to n}\|$$

This number is nonnegative (because the norm is ≥ 1) and depends on E and the parameters of the potential. From γ_n we obtain, as $n \to \pm\infty$,

$$\overline{\gamma}_\pm = \limsup_{n \to \pm\infty} \gamma_n \quad , \quad \underline{\gamma}_\pm = \liminf_{n \to \pm\infty} \gamma_n$$

We find the same numbers by using the trace- or any other norm. In fortunate cases the limits exist (i.e., lim sup and lim inf coincide) and give $\gamma_\pm = \gamma_\pm(E, V)$. These we call the Lyapunov exponents. If $\gamma_+ = \gamma_-$, the common value is denoted by $\gamma(E, V)$.

To elucidate the meaning of the Lyapunov exponent, recall that

$$\|T_{1 \to n}\|_2^2 = \|\Psi_n^1\|^2 + \|\Psi_n^2\|^2$$

cf. equations (3.1), (3.2) and (3.5). Let, e.g., $n \to +\infty$ and suppose that γ_+ exists. If $\gamma_+ = 0$, every solution is subexponential. Suppose that $\gamma_+ > 0$. Then asymptotically

$$\ln \|\Psi_n^i\| \asymp n\gamma_+$$

for $i = 1$ or 2 or both and, since any solution is a linear combination of the two standard ones, the same asymptotics is valid for all solutions, except perhaps a unique one (which is asymptotically smaller). The Multiplicative Ergodic Theorem due to Osceledec [104] and Ruelle [123] asserts that there is indeed a unique solution ψ with an exponential decay:

$$\ln \|\Psi_n\| \asymp -n\gamma_+$$

If both of $\gamma_\pm$ are positive, it may happen that the unique solution decaying exponentially to the left coincides with the unique solution decaying exponentially to the right: we have an exponentially localized state. If this is not the case, for the given energy all solutions increase exponentially at least in one direction. Such an energy is considered as 'physically forbidden' and the solution physically irrelevant, because there can be no electronic state inside the solid, corresponding to it.

Let us make this statement somewhat more explicit. We may ask: Provided that the electron is in the interval $[-L, L]$, what is the probability of finding it at site n? The answer is $|\psi_n|^2 / \sum_{k=-L}^{L} |\psi_k|^2$. This number is of the order of unity close to L or $-L$ and exponentially decaying towards the inside. So in any finite sample, at the given energy, the electron cannot penetrate into the bulk, it is exponentially localized at the boundaries. Also, one can learn from generalized eigenfunction expansion that solutions increasing faster than any power of $|n|$ will not appear in the expansion of wave packets or computation of matrix elements and are therefore of no relevance to Physics.

3.4 Scattering problem: Landauer resistance

Suppose we have a finite sample: a potential given at $n = 1, ..., L$. Our aim is to discuss scattering of an electron of energy E on the sample. We devise our scattering experiment so as to have access to all energies. To this end, the potential is extended to $\mathbf{Z}$ with constant values,

$$V_n = \begin{cases} \omega_1 & \text{if } n \leq 0 \\ \omega_2 & \text{if } n > L \end{cases}$$

chosen so that $|\omega_1 - \omega_2| < 4$. Then the scattering problem is defined for energies satisfying the inequalities

$$|E - \omega_1| < 2 \quad , \quad |E - \omega_2| < 2$$

(Notice that $E < \omega_i$ is allowed, see the remark in the first paragraph of Section 3.1.) The general solution has the form

$$\psi_n = \begin{cases} Ae^{ik_1 n} + Be^{-ik_1 n}, & n \leq 1 \\ Ce^{ik_2 n} + De^{-ik_2 n}, & n \geq L \end{cases} \tag{3.6}$$

(the plane waves extend to $n = 1$ and $n = L$) where the real wave numbers k_i are related to E and ω_i via the equations

$$2 \cos k_i = E - \omega_i \quad , \quad i = 1, 2$$

There is no loss of generality, if we suppose that $0 < k_i < \pi$. With this convention, the scattering problem amounts to set $A = 1$, $B = r$, $C = t$ and $D = 0$ and to solve for t and r. The Landauer resistance of the sample of length L is defined as $R_L = |r|^2/|t|^2$.

ψ with the scattering boundary condition is a complex solution of the Schrödinger equation. Therefore, its complex conjugate is a linearly independent solution to the same (real) energy. The Wronskian between ψ and ψ^* is a constant times the current density: its constancy physically means current conservation. Compute the Wronskian at $n = 0$ and at $n = L$. One finds

$$W[\psi, \psi^*] = 2i(1 - |r|^2) \sin k_1 = 2i|t|^2 \sin k_2$$

so that

$$|t|^2 \sin k_2 = (1 - |r|^2) \sin k_1$$

This relation is well-known in the special case of $k_1 = k_2$. Because the sines are positive, $|r|$ cannot exceed 1.

We want to express R_L in terms of the elements a, b, c, d of the transfer matrix $T_{1 \to L}$. (Here we use the notations of Eq.(3.3)). This can be done directly by solving the linear problem

$$\begin{pmatrix} te^{ik_2(L+1)} \\ te^{ik_2 L} \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} e^{ik_1} + re^{-ik_1} \\ 1 + r \end{pmatrix}$$

but there is a more elegant way to do it. We can express the Landauer resistance also in terms of another type of transfer matrix, usually applied for the Schrödinger equation in the continuum. This transfer matrix,

$$Y = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

connects the coefficients A and B to C and D, see Eq.(3.6):

$$\begin{pmatrix} C \\ D \end{pmatrix} = Y \begin{pmatrix} A \\ B \end{pmatrix}$$

In contrast with $T_{1 \to L}$, Y depends on k_1 and k_2. Let now ψ denote the solution with $A = 1$ and $B = 0$; it follows that $C = \alpha$ and $D = \gamma$. ψ^*, the complex conjugate of ψ, is also a solution with $A = 0$ and $B = 1$ and, thus, with $C = \beta$ and $D = \delta$. We find therefore

$$\gamma = \beta^* \quad , \quad \delta = \alpha^*$$

Furthermore, the Wronskian of ψ and ψ^* computed at $n = 0$ and at $n = L$ yields

$$W[\psi, \psi^*] = 2i \sin k_1 = 2i(|\alpha|^2 - |\beta|^2) \sin k_2$$

and thus

$$\det Y = |\alpha|^2 - |\beta|^2 = \sin k_1 / \sin k_2$$

The scattering problem

$$\begin{pmatrix} t \\ 0 \end{pmatrix} = Y \begin{pmatrix} 1 \\ r \end{pmatrix}$$

trivially gives

$$r = -\beta^*/\alpha^* \quad , \quad t = \frac{1}{\alpha^*} \frac{\sin k_1}{\sin k_2} \tag{3.7}$$

from which

$$R_L = |\beta|^2 \frac{\sin^2 k_2}{\sin^2 k_1}$$

Another expression of R_L in terms of the trace norm of Y can also be obtained.

$$\|Y\|_2^2 = 2|\alpha|^2 + 2|\beta|^2 = 4|\beta|^2 + 2\frac{\sin k_1}{\sin k_2}$$

With this we find

$$R_L = \frac{1}{4}\|Y\|_2^2\frac{\sin^2 k_2}{\sin^2 k_1} - \frac{1}{2}\frac{\sin k_2}{\sin k_1}$$

These formulas are frequently used with $k_1 = k_2$, see e.g. [46], [85], [82]. It remains to connect the two different kinds of transfer matrices. This can be done by simple inspection and results

$$\begin{pmatrix} e^{ik_2(L+1)} & e^{-ik_2(L+1)} \\ e^{ik_2 L} & e^{-ik_2 L} \end{pmatrix} Y = T_{1\to L}\begin{pmatrix} e^{ik_1} & e^{-ik_1} \\ 1 & 1 \end{pmatrix}$$

Solving this equation for α and β and substituting into Eq.(3.7) we obtain

$$t = -2i\sin k_1 e^{-ik_2 L}(ae^{-ik_1} + b - e^{ik_2}(ce^{-ik_1} + d))^{-1} \tag{3.8}$$

$$r = -\frac{ae^{ik_1} + b - e^{ik_2}(ce^{ik_1} + d)}{ae^{-ik_1} + b - e^{ik_2}(ce^{-ik_1} + d)} \tag{3.9}$$

and

$$R_L(k_1, k_2) = (4\sin^2 k_1)^{-1}|ae^{ik_1} + b - ce^{i(k_1+k_2)} - de^{ik_2}|^2 \tag{3.10}$$

Recall that R_L depends on E via a, b, c, d which are real polynomials of E. The ordinary choice for the potential outside the sample is $\omega_1 = \omega_2 = 0$. With this we get $k_1 = k_2 = k$, $2\cos k = E$ and can 'test the sample' at energies between -2 and 2.

A nice and simple form is obtained for $k_1 = k_2 = \pi/2$ which corresponds to $\omega_1 = \omega_2 = E$:

$$R_L(\pi/2, \pi/2) = |ia + b + c - id|^2/4 = (\|T_{1\to L}\|_2^2 - 2)/4$$

A truly intrinsic resistance is the minimum of R_L over all k_1, k_2 which, in general, cannot be given in a closed form. The minimum over k_2, when k_1 is fixed at $\pi/2$, is still easy to find:

$$\min_{k_2} R_L(\pi/2, k_2) = R_L(\pi/2, \arg\frac{a-ib}{c-id}) = (1/4)(\sqrt{a^2 + b^2} - \sqrt{c^2 + d^2})^2$$

If the Lyapunov exponent is positive, the asymptotic behavior of the resistance is the same for all k_1, k_2: R_L grows with L like $\exp\{2\gamma_+ L\}$.

4 Schrödinger equation with periodic potentials

Periodic differential equations have a fully developed beautiful theory (Floquet theory, see e.g. [45]) which can be adapted without any difficulty to the case of difference equations. Moreover, strictly ergodic sequences are well approximated by periodic ones, and most of the results discussed in Sections 6 and 7 deeply rely upon this fact. In this section we therefore survey the periodic case.

Let the potential be periodic with period $L \geq 1$ finite:

$$V_{n+L} = V_n \quad \text{for any integer } n$$

Consequently,

$$T_{m+L\to n+L} = T_{m\to n} \quad, \text{ all } m, n$$

We exploit this by writing $n = kL + m$ where $k = k(n)$ and $0 \leq m = m(n) < L$ are uniquely determined and, e.g. for $n > 0$,

$$\Psi_n = \begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = T_{1\to n}\Psi_0 = T_{1\to m}(T_{1\to L})^k\Psi_0$$

According to the value of E we can distinguish several cases (see also Figure 1):

(1) The transfer matrix is elliptic or hyperbolic,

$$|\operatorname{tr} T_{1 \to L}(E)| = |\lambda + \lambda^{-1}| \neq 2$$

where λ and λ^{-1} are the eigenvalues. In this case there exists a matrix S (generally nonunitary) such that

$$S^{-1} T_{1 \to L} S = \begin{pmatrix} \lambda & 0 \\ 0 & \lambda^{-1} \end{pmatrix}$$

Therefore we can write

$$\Psi_n = T_{1 \to m} S \begin{pmatrix} \lambda^k & 0 \\ 0 & \lambda^{-k} \end{pmatrix} S^{-1} \Psi_0$$

The initial condition

$$\Psi_0 = S \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

yields the solution

$$\Phi_n^1 = \lambda^{k(n)} T_{1 \to m(n)} S \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

while with

$$\Psi_0 = S \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

we get

$$\Phi_n^2 = \lambda^{-k(n)} T_{1 \to m(n)} S \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Because $m(n)$ is an L-periodic function, $\lambda^{\pm k}$ in $\Phi^{1,2}$ multiplies an L-periodic function of n. There are two cases:

(1.1) The transfer matrix is elliptic,

$$\lambda = e^{i\eta} \quad , \quad \operatorname{tr} T_{1 \to L}(E) = 2\cos\eta \quad , \quad \eta \neq \text{integer} \times \pi$$

The two solutions $\phi^{1,2}$ are Bloch waves and E is in one of the (at most L) 'stability intervals'. The Lyapunov exponent exists, $\gamma_+ = \gamma_- = \gamma(E) = 0$. The Landauer resistance R_n is a bounded quasiperiodic function of n (periodic, if η is a rational multiple of π).

(1.2) The transfer matrix is hyperbolic, say, $|\lambda| > 1$. The two solutions can be written as

$$\phi_n^1 = \lambda^{\lfloor n/L \rfloor} p_n \quad , \quad \phi_n^2 = \lambda^{-\lfloor n/L \rfloor} q_n$$

with L-periodic sequences p_n, q_n. The energy is in an open - maybe semi-infinite - interval. The finite intervals are called 'forbidden gaps', they separate the stability intervals. The Lyapunov exponent $\gamma(E) = L^{-1} \ln|\lambda|$. The Landauer resistance R_n grows exponentially (with exponent 2γ).

(2) The transfer matrix is parabolic. There exists a unitary matrix U such that

$$U^{-1} T_{1 \to L} U = \begin{pmatrix} 1 & b \\ 0 & 1 \end{pmatrix} \quad , \quad b \neq 0$$

The solution can therefore be written as

$$\Psi_n = T_{1 \to m} U \begin{pmatrix} 1 & kb \\ 0 & 1 \end{pmatrix} U^{-1} \Psi_0$$

The initial condition

$$\Psi_0 = U \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

gives rise to the periodic solution

$$\Phi_n = T_{1 \to m(n)} U \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and any other solution oscillates and grows linearly with a slope b/L. The energy is a boundary point of a stability interval. The Lyapunov exponent is zero, the Landauer resistance has a quadratic increase.

(3) Accidentally it may happen that $T_{1\to L}(E) = \pm I$. Then the general solution

$$\Psi_n = T_{1\to m(n)}\Psi_0$$

is periodic for all initial conditions. This situation is quoted as the 'closure of a forbidden gap' (cf. Figure 1b). In most concrete cases, it is difficult to say whether it occurs or not. If all the gaps are open, there are $L-1$ of them, separating L disjoint stability intervals. Some examples :

(i) For the Almost-Mathieu equation with $\alpha = p/q$ rational and $q\omega/\pi$ noninteger all the $(q-1)$ gaps are open. If $\omega = 0$, p is odd and $q = 4m$, then one gap is closed (Bellissard, Simon [21], Choi, Elliot, Yui [31]).

(ii) For circle potentials (2.2) with rational α all the gaps are open.

(iii) We can obtain periodic potentials by iterating a substitution on a letter a finite number of times and repeating the result periodically. Doing this with the period-doubling substitution ($\sigma(a) = ab$, $\sigma(b) = aa$), for the resulting equation all the gaps are open (Bellissard, Bovier, Ghez [15], [27]). For the Thue-Morse substitution ($\sigma(a) = ab$, $\sigma(b) = ba$) the trace map ([9])

$$x_{n+2} - 2 = (x_{n+1} - 2)x_n^2 \qquad (n \geq 1)$$

with $x_n = \mathrm{tr}\, T_{1\to 2^n}$ reveals that x_n is a 2^n degree polynomial of E, and $x_{n+2} - 2$ has double zeros at the 2^n simple zeros of x_n. This shows (see Fig. 1) that at least one fourth of the gaps is closed! In fact, $1/4$ is the precise proportion of the closed gaps ([12]; see also [10] for the corresponding phonon problem).

(iv) For the best periodic approximations of a hierarchical potential all the gaps are open (Kunz, Livi, Sütő [90]).

We close this section with the conclusion that the physically relevant solutions belong to energies which fall into the stability intervals:

$$|\mathrm{tr}\, T_{1\to L}(E)| < 2$$

These solutions are the well-known Bloch waves. The stability intervals are nothing else than the bands in the spectrum of the periodic Schrödinger operator.

5 Spectral theory

Let us come back to the question we asked already in the previous sections. The Schrödinger equation on $\mathbf{R}^d$ or $\mathbf{Z}^d$ can be solved for any E. Which are the physically relevant solutions? What can be said about the corresponding energies? Spectral theory provides the following answer:

(i) To compute matrix elements of functions of the energy operator, it suffices to consider only the polynomially bounded solutions of the Schrödinger equation.

(ii) Every subexponential solution (growing slower than any exponential) belongs to an energy which is in the spectrum of the energy operator.

5.1 Schrödinger operator, ℓ^2-space and spectrum

Define an operator H on the sequences $\psi = \{\psi_n\}$ by

$$(H\psi)_n = \psi_{n-1} + \psi_{n+1} + V_n\psi_n$$

Then Eq.(2.1) is equivalent to $H\psi = E\psi$. We call H the Schrödinger operator; it can be represented with the infinite tridiagonal (Jacobi) matrix (denoted by the same letter)

$$H = \begin{pmatrix} \cdot & \cdot & & \cdot & & \\ & 1 & V_{n-1} & 1 & & \\ & & 1 & V_n & 1 & \\ & & & \cdot & \cdot & \cdot \end{pmatrix} \tag{5.1}$$

Consider

$$\ell^2(\mathbf{Z}) = \left\{ \psi : \sum_{n=-\infty}^{\infty} |\psi_n|^2 < \infty \right\}$$

This is a *separable* Hilbert space (it contains a countable dense set) with the inner product $(\varphi, \psi) = \sum_{n=-\infty}^{\infty} \varphi_n^* \psi_n$, and H is a selfadjoint operator on it. In what follows, we use the notation $\mathcal{H}$ for a separable Hilbert space. We call the elements of $\mathcal{H}$ *vectors*. The norm of a vector ψ is defined by $\|\psi\|^2 = (\psi, \psi)$. It should not be confounded with the norm of the $\mathbf{C}^2$ vectors which we introduced in Eq.(3.1) and denote by capital Greek letters.

Suppose, for the sake of simplicity, that V is a bounded sequence. *The spectrum $\sigma(H)$ of H is the set of E values for which $E - H$ has no bounded inverse*: One can find some vector ψ such that the equation

$$(E - H)\varphi = \psi \tag{5.2}$$

has no vector solution for φ (but may have a solution outside $\mathcal{H}$, see Problem 5.2.2) or it has more than one vector solutions. In the second case $(E - H)\varphi = 0$ has a nontrivial vector solution, that we call an *eigenvector* of H, belonging to the *eigenvalue E*. (Recall that the spectrum of a finite matrix A is the set of its eigenvalues, and

$$\det(\lambda - A) = 0 \text{ if and only if } (\lambda - A)^{-1} \text{ does not exist.)}$$

The spectrum is real, nonempty and closed, i.e., contains all of its limit points.

Example. Let us decompose H into off-diagonal and diagonal parts, $H = H_0 + V$. Then $\sigma(H_0) = [-2, 2]$. If V is L-periodic,

$$\sigma(H) = \{E : |\operatorname{tr} T_{1 \to L}(E)| \leq 2\}$$

In either cases, the Schrödinger equation has no vector solution, thus there is no eigenvalue in the spectrum.

If E is an isolated point in $\sigma(H)$, then E is an eigenvalue.

The *essential spectrum*, $\sigma_{\mathrm{ess}}(H)$, of H is the set of all non-isolated points of $\sigma(H)$, together with the isolated eigenvalues of infinite multiplicity (do not occur in one dimension). Clearly, this is a closed set. An important characterization of the essential spectrum is due to Weyl: E is in $\sigma_{\mathrm{ess}}(H)$ if and only if it is an *approximate eigenvalue* of H in the following sense. One can find a sequence φ^n of vectors such that $\|\varphi^n\| = 1$, φ^n goes to zero weakly (in $\ell^2(\mathbf{Z})$ this means that $\varphi_k^n \to 0$ for each k fixed: either φ^n spreads over larger and larger domains or it remains well localized but 'escapes' to infinity) and

$$H\varphi^n = E\varphi^n + \varepsilon^n \tag{5.3}$$

where ε^n are vectors, $\|\varepsilon^n\| \to 0$.

If ψ is not an eigenvector but it is a subexponential solution of $H\psi = E\psi$, one can construct such a 'Weyl sequence', so $E \in \sigma_{\mathrm{ess}}(H)$. If ψ is polynomially bounded, we call it a *generalized eigenvector (eigenfunction)* of H, and E a *generalized eigenvalue*.

Problem 1. Construct a Weyl sequence for a subexponential solution ψ which is not an eigenvector. *Hint:* Replace ψ_k by 0 for $k < 0$ and $k > n$ and normalize.

5.2 Point spectrum

The point spectrum of H is the set of all eigenvalues of H. It is denoted by $\sigma_{\mathrm{pp}}(H)$. The point spectrum may be empty, finite or countably infinite. The *pure point subspace* of $\mathcal{H}$ is the subspace spanned by all the eigenvectors of H. It is denoted by $\mathcal{H}_{\mathrm{pp}}$.

We say that H has a *pure point spectrum*, if its eigenvectors form a basis in the Hilbert space, that is, $\mathcal{H} = \mathcal{H}_{\mathrm{pp}}$. In this case the spectrum is the closure of the set of eigenvalues:

$$\sigma(H) = \overline{\sigma_{\mathrm{pp}}(H)} = \sigma_{\mathrm{pp}}(H) \cup \{\text{limit points of } \sigma_{\mathrm{pp}}(H)\}$$

Example. A nontrivial counterexample known for every physicist is the hydrogen atom. Here the Hilbert space is $L^2(\mathbf{R}^3)$. The energy operator of the hydrogen atom has infinitely many bound

states (eigenvectors) which, however, do not span $\mathcal{H}$. So $\mathcal{H}_{\mathrm{pp}}$ is an actual part of $\mathcal{H}$. σ_{pp} is a discrete set of negative numbers with a unique accumulation point, 0. Any $E > 0$ belongs to the spectrum but *is not* an eigenvalue, only a generalized eigenvalue. The corresponding generalized eigenvectors are bounded: they are products of a plane wave with a confluent hypergeometric function. The generalized eigenvectors ('scattering waves') can be used to build up wave packets, i.e., square integrable functions (vectors of $\mathcal{H}$) which are orthogonal to every eigenvector.

Problem 1. Find a possible Weyl sequence to show explicitly that 0 is in the essential spectrum of the energy operator of the hydrogen atom.

σ_{pp} is called a *dense point spectrum* if it is nonempty and has no isolated point. If, for a bounded recurrent potential, there is a point spectrum, it is a dense point spectrum (see Problem 6.2.2).

Examples of dense pure point spectra

1. Let $H = V$, i.e., a diagonal matrix with $V_n = \cos 2\pi n\alpha$, where α is irrational. V has a pure point spectrum, dense in $[-1, 1]$:

$$\sigma_{\mathrm{pp}}(V) = \{V_n\}_{n=0}^\infty \quad , \quad \sigma(V) = [-1, 1]$$

The eigenvector belonging to the eigenvalue V_n is δ^n, the unit vector concentrated on the site n. The set of eigenvectors is the canonical basis in $\ell^2(\mathbf{Z})$.

Problem 2. Choose E in $[-1, 1]$ but $E \neq V_n$, any n. Use the definition of the spectrum to show that $E \in \sigma(V)$.

2. Anderson localization. Let V_n be identically distributed independent random variables. Let $V(\omega) = \{V(\omega)_n\}$ denote a realization, $H(\omega) = H_0 + V(\omega)$.

(i) Pastur [106]: There exists a set $\Sigma \subset \mathbf{R}$ such that

- $\sigma(H(\omega)) = \Sigma$ with probability 1.

- Σ contains no isolated points.

- Any $E \in \Sigma$ is *not* an eigenvalue with probability 1.

(ii) Kunz, Souillard [91](simplified): Let the probability distribution $r(x)$ of the V_n's be continuous, and $r(x) \neq 0$ if and only if $a < x < b$. Then

- the spectrum of $H(\omega)$ is pure point with probability 1.

- $\Sigma = [a - 2, b + 2]$

- All the eigenvectors are exponentially localized.

(iii) Carmona, Klein, Martinelli [28]: Let V_n be Bernoulli-distributed,

$$V_n = \begin{cases} 0 & \text{with probability } p \\ b & \text{with probability } 1 - p \end{cases}$$

Then the spectrum is pure point with probability 1,

$$\Sigma = [-2, 2] \cup [b - 2, b + 2]$$

and all the eigenvectors are exponentially localized.

3. Almost Mathieu equation ($\lambda > 0$).

Choose ω at random in the interval $[0, 1)$ (according to the uniform distribution). There is an appealing nonrigorous argument (Aubry-André duality, [4]), according to which the spectrum should be pure point for $\lambda > 2$. This is not quite true, but seems to hold for good Diophantine α and almost every ω:

(i) If α is irrational, the spectrum is independent of ω, $\sigma(H(\omega)) = \Sigma(\alpha, \lambda)$.

(ii) Sinai [131], Fröhlich, Spencer and Wittwer [50]: If α is a good Diophantine number, namely, there exists some constant $c > 0$ such that

$$\min\{n\alpha - \lfloor n\alpha \rfloor, \lceil n\alpha \rceil - n\alpha\} \geq c/n^2 \quad \text{for all} \ \ n \neq 0 \tag{5.4}$$

and $\lambda \gg 1$, the spectrum of $H(\omega)$ is pure point for almost every ω and the eigenvectors decay exponentially. Sinai's proof yields also that $\Sigma(\alpha, \lambda)$ is a Cantor set (see below).

Aubry, André [4], Thouless [138], [139]: The Lebesgue measure m of the spectrum is positive,

$$m(\Sigma(\alpha, \lambda)) \geq 2|\lambda - 2| \ , \ \frac{m(\Sigma(\alpha, \lambda))}{E_u - E_l} \geq \frac{\lambda - 2}{\lambda + 2}$$

(E_u and E_l are the upper and lower boundary of the spectrum, respectively.) Recently it was shown by Last ([93], [94]) that for good Diophantine α, as for example in (5.4),

$$m(\Sigma(\alpha, \lambda)) = 2|\lambda - 2|$$

(iii) Jitomirskaya [69], [70] brought sensible improvements to the above results. She simplified the proof, weakened the Diophantine condition on α, put an explicit bound on λ ($\lambda > 15$), and showed that for all $\lambda > 2$ and for almost every ω the closure of the point spectrum has the same Lebesgue measure as the spectrum itself.

(iv) One may think that there is only some technical difficulty to extend the above results on localization from a.e ω to *every* ω. This is not true: Recently, Jitomirskaya and Simon [71] proved that for any $\lambda > 2$ and irrational α there is an uncountable set of ω's which is dense in the interval $[0, 1]$ (i.e., any point in $[0, 1]$ is a limit point of this set) and for which the spectrum of $H(\omega)$ is purely singular continuous (see later). Clearly, this set is of zero Lebesgue measure, if for the given λ and α localization occurs for a.e. ω. This result provides an example of a singular continuous measure the support of which is a thick (positive-measured) Cantor set.

5.3 Cantor sets

Take a closed interval C_0 of the real line. Cut off a finite number of open intervals which have no common boundary points with each other and with C_0. What remains is a closed set C_1 without isolated points: a union of a finite number of closed intervals. Repeat the same procedure with C_1 to obtain C_2, and so on: continue it indefinitely, by following the rule that no interval is left untouched. Let C denote the resulting set. It has the following properties:

1. C is closed. Indeed, each C_n is closed, $C_0 \supset C_1 \supset \cdots$, therefore $C = \cap_{n=0}^{\infty} C_n$, and any intersection of closed sets is closed.

2. C is nonempty. Clearly, the boundary points c_{ni} of C_n are not removed during the construction, therefore C contains them for all n.

3. There can be no interval in C, according to the construction rule.

4. There is no isolated point in C. In fact, it is clear from the construction, that the set of points c_{ni} is dense in C.

A set with the above four properties is called a Cantor set. The boundary points of C^c, the complement of the Cantor set C, form a countable dense set in C, but the Cantor set itself is uncountable. C^c is an infinite union of open intervals, the closure of which is the whole real line. What is the Lebesgue measure of C? Suppose that $m(C_{n+1}) = x_n m(C_n)$, then

$$m(C) = m(C_0) \prod_{n=0}^{\infty} x_n$$

This number is greater than zero if and only if

$$\sum_{n=0}^{\infty} \ln x_n > -\infty$$

which is true if and only if

$$\sum_{n=0}^{\infty} (1 - x_n) < \infty$$

For Cantor's 'middle thirds' set $x_n = 2/3$ and thus the Lebesgue measure is zero.

5.4 Continuous spectrum

Let $\mathcal{H}_{\text{cont}} = \mathcal{H}_{\text{pp}}^{\perp}$, the subspace orthogonal to $\mathcal{H}_{\text{pp}}$. By definition, H has no eigenvector in $\mathcal{H}_{\text{cont}}$. If the only element of $\mathcal{H}_{\text{cont}}$ is the null vector, the spectrum is pure point. If $\mathcal{H}_{\text{cont}}$ contains a nonzero vector, H has (also) a continuous spectrum $\sigma_{\text{cont}}(H)$. Indeed, the restriction of H to $\mathcal{H}_{\text{cont}}$, denoted by $H|\mathcal{H}_{\text{cont}}$, is a selfadjoint operator whose spectrum is nonempty, and

$$\sigma_{\text{cont}}(H) = \sigma(H|\mathcal{H}_{\text{cont}})$$

As a matter of fact, the dimension of $\mathcal{H}_{\text{cont}}$ is either 0 or infinite ($\mathcal{H}_{\text{cont}}$ is an H-invariant subspace ($H\mathcal{H}_{\text{cont}} \subset \mathcal{H}_{\text{cont}}$), and H has eigenvectors in any finite dimensional invariant subspace) and in the second case $\sigma_{\text{cont}}(H)$ is a nonempty closed set without isolated points. Thus we have the decomposition

$$\mathcal{H} = \mathcal{H}_{\text{pp}} \oplus \mathcal{H}_{\text{cont}} \qquad , \qquad \sigma(H) = \overline{\sigma_{\text{pp}}(H)} \cup \sigma_{\text{cont}}(H)$$

but notice that the closure of σ_{pp} (even σ_{pp} itself) may overlap with σ_{cont}.

Just as to the points of $\sigma_{\text{pp}}(H)$ there correspond the H-eigensubspaces of $\mathcal{H}_{\text{pp}}$, to certain uncountable subsets of $\sigma_{\text{cont}}(H)$ there correspond infinite-dimensional H-invariant subspaces of $\mathcal{H}_{\text{cont}}$. The connection is made by spectral projections.

5.5 Spectral projections

If H has a pure point spectrum, it can be decomposed as

$$H = \sum_{E \in \sigma_{\text{pp}}(H)} E P(\{E\})$$

where $P(\{E\})$ is the orthogonal projection to the eigensubspace belonging to the eigenvalue E (for the one dimensional Schrödinger operator all these subspaces are one dimensional). The orthogonal projections are selfadjoint and idempotent,

$$P(\{E\})^{\dagger} = P(\{E\}) = P(\{E\})^2$$

The orthogonality of the eigensubspaces belonging to different eigenvalues can be expressed as

$$P(\{E\})P(\{E'\}) = \delta_{E,E'} P(\{E\})$$

and, if the spectrum is pure point,

$$\sum_{E \in \sigma_{\text{pp}}(H)} P(\{E\}) = I = \text{ identity}$$

Physicists' notation:

If E is a nondegenerate eigenvalue, ψ the normalized eigenvector, then

$$P(\{E\}) = |\psi\rangle\langle\psi|$$

If E is degenerate,

$$P(\{E\}) = \sum |\psi^i\rangle\langle\psi^i|$$

where one has to sum over an orthonormal basis in the eigensubspace.

In general, there is a fundamental relation between certain subsets of the spectrum and orthogonal projections to H-invariant subspaces. Let $\Delta = (a, b]$ be a half-open interval of the real line, χ_Δ its characteristic function, i.e., $\chi_\Delta(E) = 1$ if $E \in \Delta$ and 0 otherwise. This function satisfies

$$\chi_\Delta(E) = \chi_\Delta(E)^* = \chi_\Delta(E)^2 \tag{5.5}$$

One can define an operator $\chi_\Delta(H)$ (formally obtained by substituting E with H) as a strong limit (see below) of polynomials of H, which inherits the properties (5.5) of the real-valued function χ_Δ and is, therefore, an orthogonal projection; we denote it by $P(\Delta)$. Similarly, orthogonal projections

can be defined for more complicated sets, called Borel sets, as, for example, countable unions and intersections of half-open intervals (closed and open sets are Borel sets), and the family of the corresponding projections have nice algebraic properties:

$$P(\emptyset) = 0 , \ P(\mathbf{R}) = I$$

$$P(\Delta_1 \cap \Delta_2) = P(\Delta_1)P(\Delta_2)$$

and for Δ_1 and Δ_2 disjoint sets

$$P(\Delta_1 \cup \Delta_2) = P(\Delta_1) + P(\Delta_2)$$

The last equality holds also in a stronger form: If Δ_i, $i = 1, 2, ...$ is an infinite sequence of pairwise disjoint Borel sets then

$$P(\cup_{i=1}^{\infty}\Delta_i) = \text{s-lim} \sum_{i=1}^{N} P(\Delta_i)$$

The sum converges in the strong sense, that is, for any $\varphi \in \mathcal{H}$

$$\sum_{i=1}^{N} P(\Delta_i)\varphi \to P(\cup_{i=1}^{\infty}\Delta_i)\varphi \ \text{ as } \ N \to \infty$$

The above properties of P are characteristic to probability measures; the only difference is that $P(\Delta)$ are operators, so P is a projection-valued probability measure. This measure is called the *(spectral) resolution of the identity*, its values on Borel sets are the *spectral projections*.

The spectral projections live on the spectrum of H:

$$P(\Delta) = P(\Delta \cap \sigma(H))$$

If $P(\Delta) \neq 0$, the linear subspace $P(\Delta)\mathcal{H}$ is nontrivial and invariant under H (because H commutes with $P(\Delta)$).

Consider now the converse relation: Let $\mathcal{A}$ be an H-invariant (closed) subspace and denote $[\mathcal{A}]$ the orthogonal projection onto $\mathcal{A}$. $[\mathcal{A}]$ may not be a spectral projection. For example, if ψ is an eigenvector belonging to a degenerate eigenvalue E and $\mathcal{A}$ is the one-dimensional subspace spanned by ψ, $[\mathcal{A}] = |\psi\rangle\langle\psi|$ is not a spectral projection. The smallest spectral projection larger than $[\mathcal{A}]$ is $P(\{E\})$ (for projections Q_1, Q_2, $Q_1 < Q_2$ means $Q_1\mathcal{H} \subset Q_2\mathcal{H}$). Similar situation may occur in the continuous spectrum. The operator H is called *multiplicity free* if the orthogonal projection onto any H-invariant subspace is a spectral projection. Clearly, $[\mathcal{H}_{\text{pp}}]$ and $[\mathcal{H}_{\text{cont}}]$ are always spectral projections:

$$[\mathcal{H}_{\text{pp}}] = P(\sigma_{\text{pp}}(H)) \ \text{ and } \ [\mathcal{H}_{\text{cont}}] = P(\sigma(H) \setminus \sigma_{\text{pp}}(H))$$

Further important examples will be given later.

For any vector ψ one can define a real positive measure μ_ψ by setting

$$\mu_\psi(\Delta) = (\psi, P(\Delta)\psi) = \|P(\Delta)\psi\|^2$$

for Borel sets Δ. This is called the *spectral measure associated with* ψ. Spectral measures play an important role in the computation of averages and transition amplitudes: The matrix elements of functions of the energy operator can be obtained as integrals with respect to these measures. The spectral projection

$$P_E = P((-\infty, E])$$

is a monotonically increasing function of E in the sense that for $E_1 < E_2$

$$P_{E_2} - P_{E_1} = P((E_1, E_2]) \geq 0$$

($P \geq 0$ means $(\psi, P\psi) \geq 0$ for all $\psi \in \mathcal{H}$, which holds because $(\psi, P\psi) = (P\psi, P\psi)$.) Therefore, with

$$\mathrm{d}P_E = P_{E+\mathrm{d}E} - P_E = P((E, E + \mathrm{d}E])$$

one can write down the spectral decomposition of H in the general case:

$$H = \int E \mathrm{d}P_E$$

This equation has the following meaning. For any $\psi \in \mathcal{H}$ and any function f, continuous on $\sigma(H)$,

$$(\psi, f(H)\psi) = \int f(E)\mathrm{d}\mu_\psi(E)$$

where

$$\mu_\psi(E) = \mu_\psi((-\infty, E]) = \|P_E \psi\|^2$$

This function increases monotonically with E and is upper semicontinuous (in jumps takes on the higher value). It fully determines the spectral measure μ_ψ. In the above equation the integration is done with this measure.

Here we open a parenthesis on measures. The main line of the discussion continues in Section 5.8.

5.6 Measures

Let $\mu(x)$ be a real monotonically increasing upper semicontinuous function on $\mathbf{R}$, finite at any finite x. With this function is associated a measure on the Borel sets Δ of $\mathbf{R}$:

$$\mu(\Delta) := \int_\Delta \mathrm{d}\mu(x) = \int \chi_\Delta(x)\mathrm{d}\mu(x)$$

which is nothing else than the total variation (increase) of μ on Δ, written as the Stieltjes-Lebesgue integral of $\chi_\Delta(x)$ with respect to $\mu(x)$. (The notation should not confound the reader: μ with a real number argument means the function, with a set argument the measure. In this way, $\mu(x) = \mu((-\infty, x])$ and $\mu(\{x\})$ is the measure of the one-point set $\{x\}$.) The set function thus obtained satisfies, indeed, the properties of (positive) measures, namely, it is nonnegative, vanishing on the empty set and countably additive:

$$\mu(\cup_{i=1}^\infty \Delta_i) = \sum_{i=1}^\infty \mu(\Delta_i)$$

if the Δ_i are pairwise disjoint sets.

Conversely, a positive measure μ which is finite on the semi-infinite intervals $(-\infty, x]$ can be used to define a monotonically increasing upper semicontinuous function, denoted also by μ, by setting

$$\mu(x) := \mu((-\infty, x])$$

This is called the *distribution function* of the measure μ.

One can define the derivative of the measure μ with respect to the Lebesgue measure at the point x as

$$\frac{\mathrm{d}\mu}{\mathrm{d}m}(x) = \lim_{J\downarrow x} \mu(J)/m(J) \le \infty$$

provided the limit exists. The limit is taken on open intervals containing x and shrinking to x. If the distribution function is continuous and differentiable at x (perhaps with infinite derivative) then its derivative $\mu'(x) = (\mathrm{d}\mu/\mathrm{d}m)(x)$. Oppositely, if $(\mathrm{d}\mu/\mathrm{d}m)(x)$ *finitely* exists then $\mu(x)$ is continuous and differentiable at x and $\mu'(x) = (\mathrm{d}\mu/\mathrm{d}m)(x)$. In the points of discontinuity of $\mu(x)$, $\mu'(x)$ does not exist, but $(\mathrm{d}\mu/\mathrm{d}m)(x)$ exists and is infinite. The set

$$S = \{x : (\mathrm{d}\mu/\mathrm{d}m)(x) \text{ does not exist finitely or infinitely}\}$$

is a part of the set where $\mu'(x)$ does not exist. Therefore we can apply a theorem ([124], Ch. IV, Theorem 9.1), valid for functions which are locally of bounded variation (like $\mu(x)$), to conclude

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that both the μ and the Lebesgue (m-) measure of S is vanishing, so $(\mathrm{d}\mu/\mathrm{d}m)(x)$ is well-defined apart from a set of zero μ- and Lebesgue measure.

Let A be a Borel set. We say that a measure μ *is concentrated on A* if $\mu(A^c) = 0$ ($A^c = \mathbf{R} \setminus A$, the complement of A). The smallest closed set on which μ is concentrated is the *support* of μ, $\mathrm{supp}\,\mu$. So if μ is concentrated on A then $\mathrm{supp}\,\mu \subset \overline{A}$, the closure of A.

An $x \in \mathbf{R}$ is a *point of increase* of the distribution function μ if for every $\varepsilon > 0$, $\mu(x + \varepsilon) > \mu(x - \varepsilon)$.

Problem 1. $\mathrm{supp}\,\mu$ is the set of points of increase of $\mu(x)$.

A Borel set A is called an *essential support* of μ if $\mu(A^c) = 0$ and for any $A_0 \subset A$ such that $\mu(A_0) = 0$, $m(A_0) = 0$ as well. So the support is unique and closed, the essential support is unique only apart from sets of zero μ- and Lebesgue measure and is normally not closed. Countable unions and intersections of essential supports are essential supports. An essential support may not be a subset of the support. An example is $A \cup B$ where A is an essential support and B a nonempty Borel set with $m(B) = 0$ and $B \cap \mathrm{supp}\,\mu = \emptyset$. However, if A is an essential support then $A \cap \mathrm{supp}\,\mu$ is again an essential support, the closure of which is the support.

It follows from the definitions, that any measure μ has an essential support on which $(\mathrm{d}\mu/\mathrm{d}m)(x)$ exists (maybe infinite).

Any measure μ can be decomposed into pure point and continuous part, $\mu = \mu_{\mathrm{pp}} + \mu_{\mathrm{cont}}$. These are respectively characterized by the equations

$$\mu_{\mathrm{pp}}(\mathbf{R}) = \sum_i \mu_{\mathrm{pp}}(\{x_i\})$$

that is, μ_{pp} is concentrated on a countable set of points, and

$$\mu_{\mathrm{cont}}(\{x\}) = \lim_{\varepsilon \downarrow 0} \mu([x - \varepsilon, x + \varepsilon]) = 0,$$

the μ_{cont}-measure of every $x \in \mathbf{R}$ is zero. If the function μ is continuous, the corresponding measure is purely continuous; if it makes jumps of heights a_i in the points x_i,

$$\mathrm{d}\mu_{\mathrm{pp}}(x) = \sum_i a_i \delta(x - x_i)\mathrm{d}x \tag{5.6}$$

For μ_{pp} there exists a smallest essential support: the set of all points of discontinuity of the function μ.

If μ and ν are two measures, we say that μ is *absolutely continuous* with respect to ν, and write $\mu \ll \nu$, if $\mu(\Delta) = 0$ whenever $\nu(\Delta) = 0$. In words, if ν is concentrated on a set, then μ is concentrated on the same set. If μ and ν vanish on the same Borel sets, i.e., they are mutually absolutely continuous, we call them *equivalent*, and write $\mu \sim \nu$. Equivalent measures have the same support and essential supports. Most often $\nu = m$, the Lebesgue measure. If we say only that μ is absolutely continuous, we mean it with respect to the Lebesgue measure. Clearly, if μ is absolutely continuous, it is continuous.

Problem 2. If two measures are absolutely continuous and have a common essential support then they are equivalent.

Problem 3. Find an absolutely continuous and a pure point measure whose supports are not essential supports. Find a measure, whose support is the smallest essential support.

A function f defined on $\mathbf{R}$ is said to be *absolutely continuous* on a finite or infinite interval J if to every $\varepsilon > 0$ there exists a $\delta > 0$ such that for any finite collection of disjoint open subintervals $(a_1, b_1), (a_2, b_2), ..., (a_n, b_n)$ of J

$$\sum_i |f(b_i) - f(a_i)| < \varepsilon \quad \text{whenever} \quad \sum_i (b_i - a_i) < \delta \tag{5.7}$$

Since δ does not depend on n, the property holds also if the number of intervals is infinite.

Problem 4. A measure is absolutely continuous if and only if its distribution function is absolutely continuous on every finite interval.

We say that two measures μ and ν are *mutually singular*, and write $\mu \perp \nu$, if there are disjoint Borel sets A and B such that μ is concentrated on A and ν is concentrated on B. Most often $\nu = m$ and we simply say that μ is singular. Any pure point measure is obviously singular.

Problem 5. Any essential support of a singular measure is of zero Lebesgue measure.

A measure is said to be *singular continuous* (with respect to the Lebesgue measure) if it is singular and continuous. An example is given in the next subsection. Thus, μ has the following decompositions into pairwise mutually singular measures:

$$\mu = \mu_{\mathrm{pp}} + \mu_{\mathrm{cont}} = \mu_{\mathrm{ac}} + \mu_{\mathrm{sing}} = \mu_{\mathrm{ac}} + \mu_{\mathrm{sc}} + \mu_{\mathrm{pp}}$$

Problem 6. Show that any measure uniquely determines its *pp, ac* and *sc* parts.

According to the value of $(\mathrm{d}\mu/\mathrm{d}m)(x)$, one can find essential supports for the different components as follows (taken over from Gilbert and Pearson [52]). Let

$$B = \{x \in \mathbf{R} : (\mathrm{d}\mu/\mathrm{d}m)(x) \text{ exists}, 0 \le (\mathrm{d}\mu/\mathrm{d}m)(x) \le \infty\}$$

The sets $M, M_{\mathrm{ac}}, M_{\mathrm{sing}}, M_{\mathrm{sc}}, M_{\mathrm{pp}}$ defined below are essential supports respectively for $\mu, \mu_{\mathrm{ac}}, \mu_{\mathrm{sing}}, \mu_{\mathrm{sc}}, \mu_{\mathrm{pp}}$:

$$
\begin{aligned}
M &= \{x \in B : 0 < (\mathrm{d}\mu/\mathrm{d}m)(x) \le \infty\} \\
M_{\mathrm{ac}} &= \{x \in B : 0 < (\mathrm{d}\mu/\mathrm{d}m)(x) = \mu'(x) < \infty\} \\
M_{\mathrm{sing}} &= \{x \in B : (\mathrm{d}\mu/\mathrm{d}m)(x) = \infty\} \\
M_{\mathrm{sc}} &= \{x \in B : (\mathrm{d}\mu/\mathrm{d}m)(x) = \infty, \ \mu(\{x\}) = 0\} \\
M_{\mathrm{pp}} &= \{x \in B : (\mathrm{d}\mu/\mathrm{d}m)(x) = \infty, \ \mu(\{x\}) > 0\}
\end{aligned}
$$

Obviously, $M_{\mathrm{ac}}, M_{\mathrm{sc}}$ and M_{pp} are pairwise disjoint sets. They are subsets of $\operatorname{supp}\mu$ and $M_{\mathrm{pp}} \subset \operatorname{supp}\mu_{\mathrm{pp}}$ (M_{pp} is the smallest essential support of μ_{pp}), but $M_{\mathrm{ac}}, M_{\mathrm{sing}}$ and M_{sc} may not be parts of the supports of the respective measures. As mentioned earlier, by intersecting them with the corresponding supports, we still get essential supports. It may happen, however, that M_{ac} is nonempty but $\mu_{\mathrm{ac}} = 0$: surely this is the case if $m(M_{\mathrm{ac}}) = 0$; or M_{sc} is nonempty, even uncountable, but $\mu_{\mathrm{sc}} = 0$. For more details see [52].

5.7   Cantor function

The Cantor function is a continuous monotonically increasing function which grows from 0 to 1 exclusively in the points of the middle-thirds Cantor set

$$C = \{\sum_{n=1}^{\infty} 3^{-n}x_n : \ x_n = 0 \text{ or } 2\}$$

In the interval $[0, 1]$ it is given by the formula

$$\alpha(x) = \sum_{n=1}^{\infty} 2^{-n-1}x_n \ \text{ if } \ x = \sum_{n=1}^{\infty} 3^{-n}x_n \ , \ \ x_n \in \{0, 1, 2\}$$

with the remark that triadic rationals are taken with their infinite representation. More interesting, it is entirely determined by the conditions

1. $2\alpha(x) = \alpha(3x) , \ 0 \le x \le 1/3$

2. $\alpha(x) + \alpha(1 - x) = 1$

3. $\alpha(x)$ is monotonically increasing

4. $\alpha(x) = 0$ if $x < 0$ and $\alpha(x) = 1$ if $x > 1$

from which the moments or the Fourier transform of α can be computed. For example, the latter is

$$\int e^{itx}\mathrm{d}\alpha(x) = e^{it/2} \prod_{n=1}^{\infty} \cos t/3^n$$

The function is represented by a 'devil's staircase'. The measure α is singular continuous, because it is continuous and its support, C, is of zero Lebesgue measure. Observe that the Fourier transform does not tend to zero when $|t|$ goes to infinity (check it with $t = 2\pi 3^k$) as it would do if α were absolutely continuous.

The support of a singular continuous measure may have positive Lebesgue measure. Define, for example, an odd function $(\mu(-x) = -\mu(x))$ on $\mathbf{R}$ by setting

$$\mu(x) = \sum_{q=1}^{\infty} 2^{-q} \sum_{p=0}^{\infty} 2^{-p} \alpha(x - p/q) \qquad \text{if } x \geq 0$$

This is a continuous function increasing in every point of $\mathbf{R}$: $\mu(x + \varepsilon) - \mu(x) > 0$ for every real x and positive ε. $\mu(x)$ is therefore the distribution function of a continuous measure μ whose support is $\mathbf{R}$. Furthermore, $\cup_{r \in \mathbf{Q}}(C + r)$ is a Borel set (a countable union of closed sets) of zero Lebesgue measure and is an essential support for μ; thus, μ is singular continuous. This situation may occur for Schrödinger operators with unbounded potentials. If $V_n = \tan n\alpha$ and α is a Liouville number (an irrational number which is extremely well approximated by rationals), all the spectral measures are purely singular continuous, and there are spectral measures the support of which is $\mathbf{R}$ ([130]).

Problem 1. Give an example of a pure point and a singular continuous measure having a common essential support.

5.8   Spectral measures and spectral types

In the comparison of two measures, μ and ν, yielding $\mu \ll \nu$, $\mu \sim \nu$ or $\mu \perp \nu$, either or both can be projection-valued, and a projection-valued measure has support, essential support and uniquely determined *pp, ac* and *sc* parts, like real measures. In particular, for any vector ψ, $\mu_\psi \ll P$, where P is the spectral resolution of the identity. Similar relations for the *pp, ac, sc* parts will be written down below. Let us start with the decomposition of the spectral resolution of the identity:

$$P = P_{\text{pp}} + P_{\text{cont}} = P_{\text{ac}} + P_{\text{sing}} = P_{\text{pp}} + P_{\text{ac}} + P_{\text{sc}}$$

Is it true that the different terms are *spectral* projection-valued measures? The answer is yes, but for the moment it is not even clear that $P_{\text{ac}}(\Delta)$ and $P_{\text{sc}}(\Delta)$ project onto H-invariant subspaces.

By definition,

$$P_{\text{pp}}(\Delta) = \sum_{E \in \Delta \cap \sigma_{\text{pp}}(H)} P(\{E\}) = P(\Delta \cap \sigma_{\text{pp}}(H))$$

which is a spectral projection. The smallest essential support of P_{pp} is $\sigma_{\text{pp}}(H)$. Notice that

$$P_{\text{pp}}(\Delta) = P(\sigma_{\text{pp}}(H))P(\Delta) = [\mathcal{H}_{\text{pp}}]P(\Delta)$$

where the two projections commute. Let $\psi \in \mathcal{H}_{\text{pp}}$. Then

$$\mu_\psi(\mathbf{R}) = \|\psi\|^2 = \|P_{\text{pp}}(\mathbf{R})\psi\|^2 = \sum_{E \in \sigma_{\text{pp}}(H)} \mu_\psi(\{E\})$$

i.e., μ_ψ is a pure point measure and $\mu_\psi \ll P_{\text{pp}}$.

Also, by definition, for any Borel set Δ,

$$P_{\text{cont}}(\Delta) = P(\Delta) - \sum_{E \in \Delta \cap \sigma_{\text{pp}}(H)} P(\{E\}) = P(\Delta \setminus \sigma_{\text{pp}}(H))$$

is a spectral projection. The support of P_{cont} is $\sigma_{\text{cont}}(H)$. Notice that

$$P_{\text{cont}}(\Delta) = (I - [\mathcal{H}_{\text{pp}}])P(\Delta) = [\mathcal{H}_{\text{cont}}]P(\Delta) = P(\sigma_{\text{pp}}(H)^c)P(\Delta)$$

where the two projections commute. Let $\psi \in \mathcal{H}_{\text{cont}}$. Then for any $E \in \mathbf{R}$

$$\mu_\psi(\{E\}) = \|P(\{E\})\psi\|^2 = \|P(\{E\})[\mathcal{H}_{\text{cont}}]\psi\|^2 = \|P_{\text{cont}}(\{E\})\psi\|^2 = 0$$

i.e., μ_ψ is purely continuous and $\mu_\psi \ll P_{\text{cont}}$.

A purely continuous spectral measure can still be decomposed into absolutely and singular continuous parts. We would like to perform the analogous decomposition on $\mathcal{H}_{\text{cont}}$, $\sigma_{\text{cont}}(H)$ and P_{cont}.

Problems.

1. μ_ψ is concentrated on a Borel set A if and only if $P(A)\psi = \psi$. As a consequence, if $\psi \in P(A)\mathcal{H}$, $\operatorname{supp}\mu_\psi \subset \overline{A}$.

2. $\mu_{H\psi} \ll \mu_\psi$. In particular, if μ_ψ is absolutely or singular continuous then $\mu_{H\psi}$ is absolutely or singular continuous, respectively. (*Remark.* We know already that if μ_ψ is pure point, $\mu_{H\psi}$ is also pure point because $\psi \in \mathcal{H}_{\text{pp}}$ and $H\mathcal{H}_{\text{pp}} \subset \mathcal{H}_{\text{pp}}$.)

3. If $\mu_\psi = (\mu_\psi)_{\text{pp}} + (\mu_\psi)_{\text{ac}} + (\mu_\psi)_{\text{sc}}$ then there exist orthogonal vectors ψ^{pp}, ψ^{ac} and ψ^{sc} such that $\psi = \psi^{\text{pp}} + \psi^{\text{ac}} + \psi^{\text{sc}}$ and $(\mu_\psi)_{\text{pp}} = \mu_{\psi^{\text{pp}}}$, $(\mu_\psi)_{\text{ac}} = \mu_{\psi^{\text{ac}}}$ and $(\mu_\psi)_{\text{sc}} = \mu_{\psi^{\text{sc}}}$. *Hint.* Choose disjoint essential supports and apply 1.

4. Let ψ^i be a sequence of vectors converging to a vector ψ (i.e., $\|\psi^i - \psi\| \to 0$). Suppose that μ_{ψ^i} are singular measures. Then μ_ψ is singular. *Hint.* (i) $\mu_{\psi^i} \to \mu_\psi$ on Borel sets. (ii) Let A_i be an essential support to μ_{ψ^i}, then $\cup A_i$ is an essential support to μ_ψ.

It follows from Problem 2 that the vectors generating a purely *ac* spectral measure form an H-invariant subspace $\mathcal{H}_{\text{ac}}$; similarly, the vectors giving rise to a purely *sc* spectral measure form an H-invariant subspace $\mathcal{H}_{\text{sc}}$. (That the vectors of the same pure spectral type form a *subspace* is the subject of Problem 7 below.) According to Problem 3, $\mathcal{H}_{\text{ac}}$ and $\mathcal{H}_{\text{sc}}$ are orthogonal and span $\mathcal{H}_{\text{cont}}$. Thus $\mathcal{H}_{\text{ac}}$ and $\mathcal{H}_{\text{sc}}$ are necessarily closed and

$$\mathcal{H}_{\text{cont}} = \mathcal{H}_{\text{ac}} \oplus \mathcal{H}_{\text{sc}}$$

(Problem 4 shows also explicitly that $\mathcal{H}_{\text{sc}}$ is closed.) Now we can consider the restrictions of H to $\mathcal{H}_{\text{ac}}$ and to $\mathcal{H}_{\text{sc}}$: these are selfadjoint operators, their spectra are $\sigma_{\text{ac}}(H)$ and $\sigma_{\text{sc}}(H)$, respectively. Absolutely continuous and singular continuous spectral measures are concentrated respectively on $\sigma_{\text{ac}}(H)$ and $\sigma_{\text{sc}}(H)$.

In summary, we obtained the following decompositions:

$$\mathcal{H} = \mathcal{H}_{\text{pp}} \oplus \mathcal{H}_{\text{ac}} \oplus \mathcal{H}_{\text{sc}}$$

Correspondingly, for any $\psi \in \mathcal{H}$,

$$\psi = \psi^{\text{pp}} + \psi^{\text{ac}} + \psi^{\text{sc}}$$

and

$$\mu_\psi = \mu_{\psi^{\text{pp}}} + \mu_{\psi^{\text{ac}}} + \mu_{\psi^{\text{sc}}}$$

What about the decomposition of P_{cont}? Because

$$[\mathcal{H}_{\text{cont}}] = [\mathcal{H}_{\text{ac}}] + [\mathcal{H}_{\text{sc}}]$$

where the two projections are orthogonal, we get

$$P_{\text{cont}}(\Delta) = [\mathcal{H}_{\text{cont}}]P(\Delta) = [\mathcal{H}_{\text{ac}}]P(\Delta) + [\mathcal{H}_{\text{sc}}]P(\Delta)$$

with commuting operators in the products.

Problem 5. Show that the projection-valued measures $[\mathcal{H}_{\text{ac}}]P$ and $[\mathcal{H}_{\text{sc}}]P$ are absolutely and singular continuous, respectively.

Since the decomposition of P_{cont} into *ac* and *sc* parts is unique, we obtained that

$$P_{\text{ac}} = [\mathcal{H}_{\text{ac}}]P \quad , \quad P_{\text{sc}} = [\mathcal{H}_{\text{sc}}]P \tag{5.8}$$

So $P_{\text{ac}}(\Delta)$ and $P_{\text{sc}}(\Delta)$ project onto H-invariant subspaces within $\mathcal{H}_{\text{ac}}$ and $\mathcal{H}_{\text{sc}}$, respectively. It remains to show that they are spectral projections.

Let A and B be disjoint essential supports for P_{ac} and P_{sc}, respectively, which are disjoint also from $\sigma_{\mathrm{pp}}(H)$. Then

$$[\mathcal{H}_{\mathrm{ac}}] = P_{\mathrm{ac}}(A) = P(A) \ \text{ and } \ [\mathcal{H}_{\mathrm{sc}}] = P_{\mathrm{sc}}(B) = P(B)$$

Indeed, for any $\psi \in \mathcal{H}$, $[\mathcal{H}_{\mathrm{ac}}]\psi = \psi^{\mathrm{ac}}$ while

$$
\begin{aligned}
P(A)\psi = P(A)\psi^{\mathrm{ac}} + P(A)(\psi^{\mathrm{sc}} + \psi^{\mathrm{pp}}) &= P_{\mathrm{ac}}(A)\psi + (P_{\mathrm{sc}}(A) + P_{\mathrm{pp}}(A))\psi \\
&= P_{\mathrm{ac}}(A)\psi = P_{\mathrm{ac}}(\mathbf{R})\psi = \psi^{\mathrm{ac}}
\end{aligned}
$$

The proof is similar for $[\mathcal{H}_{\mathrm{sc}}]$. The result shows that $P_{\mathrm{ac}}(\Delta)$ and $P_{\mathrm{sc}}(\Delta)$ are the spectral projections $P(A \cap \Delta)$ and $P(B \cap \Delta)$, respectively. Using Eq.(5.8) and the definition of μ_ψ, it is immediately seen that $\mu_\psi \ll P_{\mathrm{ac}}$ if $\psi \in \mathcal{H}_{\mathrm{ac}}$ and $\mu_\psi \ll P_{\mathrm{sc}}$ if $\psi \in \mathcal{H}_{\mathrm{sc}}$.

At last,

$$\sigma(H) = \overline{\sigma_{\mathrm{pp}}(H)} \cup \sigma_{\mathrm{ac}}(H) \cup \sigma_{\mathrm{sc}}(H)$$

where

$$
\begin{array}{rcl}
\sigma(H) &=& \mathrm{supp}\, P \\
\sigma_{\mathrm{pp}}(H) &=& \mathrm{ess.supp}\, P_{\mathrm{pp}} \\
\sigma_{\mathrm{ac}}(H) &=& \mathrm{supp}\, P_{\mathrm{ac}} \\
\sigma_{\mathrm{sc}}(H) &=& \mathrm{supp}\, P_{\mathrm{sc}}
\end{array}
\tag{5.9}
$$

It is also important to know, how to reconstruct the spectrum from real measures. Clearly, if μ is any real measure equivalent to P then in Eq.(5.9) P can be replaced by μ.

Problem 6. Let μ be a measure and $\mu_\psi \ll \mu$ for all $\psi \in \mathcal{H}$. Then $P \ll \mu$.

Problem 7. $\mu_{\alpha\psi^1 + \beta\psi^2} \ll \mu_{\psi^1} + \mu_{\psi^2}$.

Problem 8. Let $\psi^1, \psi^2, \ldots$ be a normalized basis in $\mathcal{H}$ and $c_i > 0$ for $i = 1, 2, \ldots$ such that $\sum_{i=1}^\infty c_i < \infty$. Then

$$P \sim \sum_{i=1}^\infty c_i \mu_{\psi^i}$$

In the particular case of $\mathcal{H} = \ell^2(\mathbf{Z})$ and H the Schrödinger operator, we have a much simpler result. Let δ^0 and δ^1 be the unit vectors concentrated on 0 and 1, respectively. Then

$$P \sim \mu_{\delta^0} + \mu_{\delta^1} \tag{5.10}$$

Call μ the measure on the right side. $\mu \ll P$ is obvious, one has to show $P \ll \mu$. Let Δ be such that $\mu(\Delta) = 0$. Then $P(\Delta)\delta^0 = P(\Delta)\delta^1 = 0$ and, as a consequence,

$$P(\Delta)H^n\delta^0 = P(\Delta)H^n\delta^1 = 0 \ \text{ for } n = 1, 2, \ldots$$

From this we can conclude that $P(\Delta) = 0$ because of the following.

Problem 9. The set of vectors $\{H^n\delta^0, H^n\delta^1\}_{n=0}^\infty$ is a basis in $\ell^2(\mathbf{Z})$.

Clearly, Eq.(5.10) holds if 0 and 1 are replaced by any two successive integers.

The sum of spectral measures is, in general, not a spectral measure.

Problem 10. $\mu_{\psi^1 + \psi^2} = \mu_{\psi^1} + \mu_{\psi^2}$ if and only if the two vectors are in orthogonal H-invariant subspaces.

Therefore, for the Schrödinger operator the right member of the relation (5.10) is not a spectral measure, in general (but it *is* a spectral measure for the free Laplacian, see Section 5.9).

If H has a pure point spectrum, and for the basis in Problem 8 we choose an orthonormal set of eigenvectors, $\sum c_i \mu_{\psi^i}$ is equal to the spectral measure belonging to $\sum \alpha_i \psi^i$, where $|\alpha_i|^2 = c_i$. It is interesting to remark, that there always exist spectral measures equivalent to P, even if the spectrum is not pure point. The construction is suggested by Problem 10. Let $\mathcal{A}$ be an H-invariant subspace. A vector $\psi \in \mathcal{A}$ is a *cyclic vector* in $\mathcal{A}$ if any $\varphi \in \mathcal{A}$ can be obtained as

$$\varphi = \lim_{N \to \infty} \sum_{n=1}^N \alpha_{Nn}(H^n\psi)$$

In this case, $\mu_\varphi \ll \mu_\psi$ for all $\varphi \in \mathcal{A}$, as one can see from Problems 2 and 7. Not all H-invariant subspaces contain cyclic vectors (a counterexample is a subspace belonging to a degenerate eigenvalue), but $\mathcal{H}$ can always be written as

$$\mathcal{H} = \oplus \mathcal{A}_i \ , \tag{5.11}$$

a finite or infinite direct sum of orthogonal H-invariant subspaces with cyclic vectors. Let ψ^i be a normalized cyclic vector in the ith subspace and $\alpha_i \neq 0$, $\sum |\alpha_i|^2 < \infty$. Any $\varphi \in \mathcal{H}$ can be written as $\varphi = \sum \beta_i \varphi^i$ where $\varphi^i \in \mathcal{A}_i$. According to Problem 10,

$$\mu_\varphi = \mu_{\Sigma \beta_i \varphi^i} = \sum |\beta_i|^2 \mu_{\varphi^i} \ll \sum |\alpha_i|^2 \mu_{\psi^i} = \mu_{\Sigma \alpha_i \psi^i}$$

and, according to Problem 6, $P \sim \mu_{\Sigma \alpha_i \psi^i}$.

The decomposition (5.11) is nonunique. We can start with any ψ^1, choose $\mathcal{A}_1$ as the smallest subspace containing $H^n \psi^1$ for every nonnegative integer n, choose any ψ^2 orthogonal to $\mathcal{A}_1$, and so on... . The smallest number of subspaces we need for the decomposition may be called the *multiplicity* of the spectrum of H. Problem 9 shows that the multiplicity of the spectrum of a Schrödinger operator on $\ell^2(\mathbf{Z})$ is 1 or 2. If the multiplicity is 1, that is, there exists a cyclic vector (in $\mathcal{H}$), H is multiplicity free also in the sense defined in 5.5.

Multiplicity may not be uniform on the spectrum, therefore it is appropriate to define it also locally: Let Δ be a Borel set such that $P(\Delta) \neq 0$, and $\mathcal{H}_\Delta = P(\Delta)\mathcal{H}$. The decomposition (5.11) can be performed on $\mathcal{H}_\Delta$, and the smallest number of subspaces we need to it is called the multiplicity of the spectrum on Δ. If Δ is an eigenvalue, we obtain the usual notion of multiplicity.

5.9   A spectral measure for H_0

Let $\mathcal{H} = \ell^2(\mathbf{Z})$, $H = H_0 = T + T^{-1}$ (recall: T is the left shift). We are going to compute explicitly μ_{δ^0}. The way to proceed is to find a measure μ such that

$$(\delta^0, H^n \delta^0) = \int E^n \mathrm{d}\mu(E) \ \text{ for all } n$$

Then we can identify μ with μ_{δ^0}.

For any unitary operator U

$$(\delta^0, H^n \delta^0) = (U\delta^0, UH^n \delta^0) = (U\delta^0, (UHU^{-1})^n U\delta^0)$$

Choose for U the Fourier transformation which maps $\ell^2(\mathbf{Z})$ onto $L^2_{\mathrm{per.}}[0,1]$: For any $\psi \in \ell^2(\mathbf{Z})$

$$(U\psi)(x) = \sum_{n=-\infty}^{\infty} \psi_n e^{2\pi i n x} \ , \quad x \in [0,1]$$

In particular, $(U\delta^0)(x) \equiv 1$ and $UT^{\pm 1}U^{-1}$ correspond respectively to the multiplication by $\exp(\mp 2\pi i x)$; therefore UHU^{-1} corresponds to the multiplication by $2\cos 2\pi x$. This gives

$$(\delta^0, H^n \delta^0) = \int_0^1 (2\cos 2\pi x)^n \mathrm{d}x = 2\int_0^{\frac{1}{2}} (2\cos 2\pi x)^n \mathrm{d}x = \int_{-2}^2 E^n \frac{\mathrm{d}E}{\pi\sqrt{4 - E^2}}$$

where we applied the substitution $E = 2\cos 2\pi x$. From here we recognize

$$\mathrm{d}\mu_{\delta^0}(E) = \begin{cases} \mathrm{d}E/\pi\sqrt{4 - E^2} & \text{if } E \in (-2, 2) \\ 0 & \text{otherwise} \end{cases}$$

By integration,

$$\mu_{\delta^0}(E) = \frac{1}{2} + \frac{1}{\pi} \arcsin(E/2) \ \text{ if } -2 \leq E \leq 2$$

and 0 below -2 and 1 above 2. This function is manifestly absolutely continuous, thus H_0 has an absolutely continuous spectrum in $[-2, 2]$. Because of the shift-invariance of H_0, $\mu_{\delta^1} = \mu_{\delta^0}$ and thus $P \sim \mu_{\delta^0}$. This shows that $\sigma(H_0) = [-2, 2]$ and the spectrum is purely absolutely continuous.

Notice that δ^0 is not a cyclic vector: $H^n\delta^0$, $n = 1, 2, \ldots$ generate only the 'even' subspace,

$$\mathcal{E} = \{\psi : \psi_{-k} = \psi_k \text{ for all } k\}$$

This subspace is H_0-invariant and the orthogonal projection onto it is not a spectral projection (cannot be written as a function of H_0 only). Therefore H_0 is not multiplicity free. In fact, the spectrum is uniformly of multiplicity 2.

5.10 $\ell^2(\mathbf{Z})$ versus $\ell^2(\mathbf{N})$

Consider the matrix (5.1) of the Schrödinger operator on $\ell^2(\mathbf{Z})$ and replace the matrix elements $H_{-1,0} = H_{0,-1} = 1$ by zeros. What kind of effect this tiny modification can have on the spectrum of the modified operator H'? According to the 'classical' Weyl theorem ([115], Vol. IV),

$$\sigma_{\mathrm{ess}}(H') = \sigma_{\mathrm{ess}}(H)$$

that is, apart from isolated eigenvalues, the two spectra coincide. The matrix of H' is of block-diagonal form, so H' can be written as $H' = H_l \oplus H_r$, where H_l and H_r are selfadjoint operators acting on $\ell^2(-\mathbf{N} \setminus \{0\})$ and $\ell^2(\mathbf{N})$, respectively. Thus,

$$\sigma(H') = \sigma(H_l) \cup \sigma(H_r)$$

For strictly ergodic potentials $\sigma_{\mathrm{ess}}(H_l) = \sigma_{\mathrm{ess}}(H_r)$, and, hence, $= \sigma_{\mathrm{ess}}(H)$.

The fate of spectral types under such a 'finite-rank' perturbation is partly uncertain. Point and singular continuous spectra may change into each other (Gordon [55], del Rio, Makarov, Simon [122]). However, the absolutely continuous spectrum is robust,

$$\sigma_{\mathrm{ac}}(H) = \sigma_{\mathrm{ac}}(H_l) \cup \sigma_{\mathrm{ac}}(H_r) \tag{5.12}$$

and this holds, whatever be the (selfadjoint) boundary condition at 0, defining H_l and H_r. The reason is that the singular spectrum is sensitive to the boundary condition at 0, while the absolutely continuous spectrum can be fully characterized by the large-time behaviour of propagating wave packets and, hence, is insensitive to local perturbations. In fact, it is stable under more general (trace class) perturbations (see e.g. [77], Chapter X, Theorem 4.4).

5.11 Asymptotic behaviour of generalized eigenfunctions. Subordinacy

We started Section 5 with a remark about the sufficiency, for Physics, of polynomially bounded solutions. This remark is based on the following deep theorem:

The spectral resolution of the identity has an essential support $\mathcal{E}$ such that for every $E \in \mathcal{E}$ there exists a solution ψ of the Schrödinger equation satisfying the following condition: For any $\delta > d/4$ (d is the space dimension), with a suitably chosen positive constant $c = c(\delta, E)$,

$$|\psi(x)| \le c(1 + |x|^2)^{\delta} \text{ for all } x \text{ in } \mathbf{R}^d \text{ or } \mathbf{Z}^d \tag{5.13}$$

The most general form of this theorem (going beyond Schrödinger operators) can be found in Berezanskii's book [22]. The Schrödinger case in the continuum, with precise conditions, assertions and proof is described in Simon's survey paper [128] (also in [29]). A simple proof for the $\ell^2(\mathbf{Z})$ case, due to Lacroix, is presented in the book of Bougerol and Lacroix [25].

Clearly, the same result is valid separately for P_{pp}, P_{ac} and P_{sc} and is nontrivial for P_{ac} and P_{sc}. It, however, does not permit to distinguish between these two cases.

It is expected that knowing the whole family of solutions for a given energy E, one can decide whether E is in the spectrum and which spectral type it belongs to. The right notion to deal with this question is *subordinacy*. It was introduced by Gilbert and Pearson [52] for the Schrödinger differential equation on the half-line, extended by Gilbert [51] to the problem on $\mathbf{R}$, and by Khan and Pearson [78] to the discrete equation on $\mathbf{N}$. A discussion of it can be found in Pearson's book [108]. Results for the equation on $\mathbf{Z}$ can be safely deduced from these works.

For a two-sided complex-valued sequence ψ and an integer N let

$$\|\psi\|_N = (\sum_{n=0}^{N}{}^* |\psi_n|^2)^{1/2}$$

The star means that for $N < 0$ the summation goes over $n = 0, -1, ..., N$. Fix E. A solution ψ of the Schrödinger equation with energy E is said to be *subordinate* at $+\infty$ $(-\infty)$ if for every linearly independent solution φ,

$$\|\psi\|_N / \|\varphi\|_N \to 0$$

as $N \to +\infty$ $(-\infty)$. Clearly, there can be at most one subordinate solution at either side, and it suffices to check the condition on a single φ linearly independent of ψ. Subordinate solutions for real energies are real.

Below, by 'solution' we mean a solution of the Schrödinger equation for given E. Consider the following sets.

- $M' = \mathbf{R} \setminus \{E \in \mathbf{R} :$ there exist two solutions, one which is subordinate at $+\infty$ but not at $-\infty$, the other which is subordinate at $-\infty$ but not at $+\infty\}$.

- $M'_{\mathrm{ac}} = \{E \in \mathbf{R} :$ every solution is nonsubordinate at $+\infty\}$
$\cup \{E \in \mathbf{R} :$ every solution is nonsubordinate at $-\infty\}$

- $M'_{\mathrm{sing}} = \{E \in \mathbf{R} :$ there exists a solution which is subordinate at $\pm\infty\}$

- $M'_{\mathrm{sc}} = \{E \in \mathbf{R} :$ there exists a solution which is subordinate at $\pm\infty$ but is not in $\ell^2(\mathbf{Z})\}$

- $M'_{\mathrm{pp}} = \{E \in \mathbf{R} :$ there exists a solution which is subordinate at $\pm\infty$ and is in $\ell^2(\mathbf{Z})\}$

Then M' is an essential support for P and $M'_{\mathrm{pp}} = \sigma_{\mathrm{pp}}(H)$. ($M'$ is the disjoint union of M'_{ac}, M'_{sc} and M'_{pp} and is a subset of $\sigma(H)$.) Furthermore, $P_{\mathrm{ac}} \neq 0$ if and only if $m(M'_{\mathrm{ac}}) > 0$, in which case M'_{ac} is an essential support for P_{ac} (and so is $M'_{\mathrm{ac}} \cap \sigma_{\mathrm{ac}}(H)$). If $P_{\mathrm{sc}} \neq 0$, M'_{sc} is an essential support for P_{sc} (and so is $M'_{\mathrm{sc}} \cap \sigma_{\mathrm{sc}}(H)$). If J is a real interval, $P_{\mathrm{ac}}(J) = P_{\mathrm{pp}}(J) = 0$ and $M'_{\mathrm{sc}} \cap J$ is an uncountable set, then $P_{\mathrm{sc}}(J) > 0$.

The above characterization shows that physicists are not quite right when saying that in the singular continuous spectrum 'all the solutions are critical'. In fact, there is one solution (the subordinate one) which is less (or more) 'critical' than the others and shows a clear analogy with an eigenvector. Notice, however, that a subordinate solution may not decay to zero at $\pm\infty$.

The union giving M'_{ac} corresponds to the union (5.12). On the intersection of the two parts of M'_{ac} the multiplicity of the spectrum is 2, otherwise it is 1 (Kac, [75], [76]).

Recently, Al-Naggar and Pearson [3] developed further the characterization of the absolutely continuous spectrum in the case of the differential equation on the half-line. Due to Eq.(5.12), their result applies to the $\ell^2(\mathbf{Z})$ case in the form presented below.

For fixed *real* E a *complex* solution ψ of the Schrödinger equation with energy E is called *rotating* at $+\infty$ $(-\infty)$ if

$$\sum_{n=0}^{N}{}^* \psi_n^2 / \sum_{n=0}^{N}{}^* |\psi_n|^2 \to 0$$

as $N \to +\infty$ $(-\infty)$. Notice that a complex solution for real E is the linear combination of two real solutions with complex coefficients. Let

$$M''_{\mathrm{ac}} = \{E \in \mathbf{R} :$$ there is a solution which is rotating at least at one of $\pm\infty\}.$$

Then, if $m(M''_{\mathrm{ac}}) > 0$, $P_{\mathrm{ac}} \neq 0$ and M''_{ac} is *inside* an essential support of P_{ac}.

Unfortunately, it is not known so far whether M''_{ac} itself is an essential support for P_{ac}.

6 Schrödinger equation with strictly ergodic potentials

6.1 Strict ergodicity

The first step is to check minimality and unique ergodicity of the sequence defining the potential. We discuss this question only briefly; the reader may consult some other lectures of this School ([1], [40], [95], [114]) and references therein. The minimality of a sequence (and then that of the hull) is equivalent to the infinite repetition, with arbitrary precision and bounded gaps, of every finite segment. In the case of sequences taking values from a finite set, once minimality is known, unique ergodicity means that the word frequencies exist (the defining limits converge).

The cosine potential of the Almost-Mathieu equation is a uniformly almost periodic sequence: For any ε there exists a sequence of integers, $\{n_i\}$, with bounded gaps such that for all i and all n

$$|V_{n+n_i} - V_n| < \varepsilon$$

(see e.g. [24]). This implies also strict ergodicity. A weaker form of almost periodicity (in the mean- or Besicovitch sense, see [24], which is equivalent to the existence of an atomic Fourier transform of the sequence, with square summable coefficients) also implies strict ergodicity. Sturmian sequences, or more generally, sequences generated by the circle map with A being the union of a finite number of intervals of the type $[a, b)$ (cf. point (2) in Sec.2) belong to this class. The Fourier coefficients of the 1-periodic function $X_A(x)$ are easy to compute. It is worth noticing that in this case the Fourier series converges everywhere but may not represent the sequence in a finite number of points. If this occurs, it is the function X_A, and not the series, which defines a strictly ergodic sequence.

Some substitutional sequences, which are not Sturmian, also admit an atomic Fourier transform. Examples are the regular paper-folding and the period-doubling sequences. As one-sided sequences, these are strictly ergodic.

In general, for every primitive substitution ξ one can build up two-sided minimal sequences, which are also uniquely (and, hence, strictly) ergodic ([56], [102]; see also [39]). The construction goes by concatenating a left- and a right-sided fixed point of some power of ξ. More precisely, one can find two letters a and b and an $n \geq 1$ such that $\xi^n(a) = \ldots a$, $\xi^n(b) = b\ldots$ and, with $\eta = \xi^n$, both $u = \eta^\infty(a) = \ldots a$ and $v = \eta^\infty(b) = b\ldots$ contain the word ab and the two-sided sequence uv is minimal and uniquely ergodic. Among others, this holds for the Thue-Morse and the Rudin-Shapiro sequences, although their Fourier transform is not atomic. Different constructions of a two-sided sequence (for example, via symmetric extension) may violate minimality (the starting sequence may not be recurrent). If both sides are related to the same substitution, the essential spectrum will not suffer, but the singular spectral measures can be seriously perturbed. (Compare with Section 5.10.)

6.2 The spectrum of $H(\omega) = H_0 + V(\omega)$

Let us start with three remarks.

1. The shift T is defined on $\ell^2(\mathbf{Z})$ by $(T\psi)_n = \psi_{n+1}$. This is a unitary operator, therefore $T^n H T^{-n}$ is unitary equivalent to and, thus, has the same spectrum as H for any finite n. This obviously holds for any potential. Notice that $TH_0T^{-1} = H_0$ and $TV(\omega)T^{-1} = V(T\omega)$, thus

$$T^n H(\omega) T^{-n} = H(T^n\omega)$$

2. If V^k is a sequence of potentials converging pointwise to a bounded potential V, then $H^k = H_0 + V^k$ tends strongly to $H = H_0 + V$, i.e., for any fixed $\psi \in \ell^2(\mathbf{Z})$, $H^k\psi \to H\psi$. Indeed,

$$\|(H^k - H)\psi\|^2 = \sum_n |V_n^k - V_n|^2 |\psi_n|^2 \to 0 \ \text{ as } k \to \infty$$

3. If the bounded selfadjoint operators H^k strongly converge to the bounded selfadjoint H and Δ is an open interval not intersecting $\sigma(H^k)$ for any k, the spectral projections $\chi_\Delta(H^k)$ also strongly converge to $\chi_\Delta(H)$ ([77], Theorem VIII.1.15); on the other hand, they all vanish and, hence, $\chi_\Delta(H) = 0$. This, however, means that Δ does not intersect $\sigma(H)$. In short,

$$\overline{\bigcup \sigma(H^k)} \supset \sigma(H) \tag{6.1}$$

Problem 1. If $V(\omega)$ is minimal, $\sigma(H(\omega))$ is independent of ω. *Hint.* Use the above remarks to prove that for any ω and ω', $\sigma(H(\omega)) \supset \sigma(H(\omega'))$ and $\sigma(H(\omega')) \supset \sigma(H(\omega))$.

The ω-independent spectrum is denoted by $\sigma(H)$.

Minimality also implies that there is no isolated point in the spectrum. Even less is sufficient:

Problem 2. If the potential is bounded and recurrent then $\sigma(H) = \sigma_{\mathrm{ess}}(H)$. *Hint.* If E is an eigenvalue and ψ the corresponding eigenvector, $\varphi^n = T^{-k_n}\psi$ with suitably chosen almost-periods k_n is a Weyl sequence.

We emphasize that the proofs of the above problems do not use ergodicity, only minimality or recurrence. This is the more interesting, because the same statements were verified for ρ-a.e. ω by using ergodicity without minimality, see Section 5.2 for the random case.

For one-dimensional ergodic potentials Pastur proved that any E is ρ-almost surely not an eigenvalue (Sec. 5.2). In fact, for this holding true, we need less than ergodicity: If Ω is a shift-invariant set of potentials and ρ is a shift-invariant probability measure on Ω, which is defined on cylinder sets, any fixed E is not in $\sigma_{\mathrm{pp}}(H(\omega))$ with ρ-probability 1. Indeed,

$$T\chi_{\{E\}}(H(\omega))T^{-1} = \chi_{\{E\}}(H(T\omega))$$

and

$$\int \mathrm{tr}\,\chi_{\{E\}}(H(\omega))\mathrm{d}\rho(\omega) = \int \sum (\delta^n, \chi_{\{E\}}(H(\omega))\delta^n)\mathrm{d}\rho(\omega)$$

$$= \sum \int (\delta^0, \chi_{\{E\}}(H(T^{-n}\omega))\delta^0)\mathrm{d}\rho(\omega) = \sum_{n=-\infty}^{\infty} \int (\delta^0, \chi_{\{E\}}(H(\omega))\delta^0)\mathrm{d}\rho(\omega)$$

All the integrals exist, the first integral takes value in $[0, 1]$ ($\chi_{\{E\}}(H(\omega)) = 0$ or it projects to a one-dimensional subspace of $\ell^2(\mathbf{Z})$) and the last sum gives 0 or ∞. The value of the first integral is therefore 0, implying $\chi_{\{E\}}(H(\omega)) = 0$ for ρ-a.e. ω.

The content of the above statement is that $\sigma_{\mathrm{pp}}(H(\omega))$ changes when ω changes. On the other hand, the closure of $\sigma_{\mathrm{pp}}(H(\omega))$ may not change:
For ergodic potentials there are closed sets Σ_{pp}, Σ_{ac} and Σ_{sc} such that

$$\overline{\sigma_{\mathrm{pp}}(H(\omega))} = \Sigma_{\mathrm{pp}}$$
$$\sigma_{\mathrm{ac}}(H(\omega)) = \Sigma_{\mathrm{ac}}$$
$$\sigma_{\mathrm{sc}}(H(\omega)) = \Sigma_{\mathrm{sc}}$$

for ρ-a.e. ω (Kunz, Souillard [91]). This theorem is the analogue of the assertion of Problem 1, but is a great deal more subtle than the constancy of the spectrum. Moreover, the result surely does not hold for *all* ω, even if the potential is strictly ergodic: a counterexample of [71] was mentioned in Section 5.2.

6.3 Integrated density of states

For finite systems the integrated density of states (IDS) as a function of E counts the number of eigenvalues per unit volume below E. Let $H_{\omega,L}^{(D)}$ denote the restriction of $H(\omega)$ to the interval $[-L, L]$ with Dirichlet boundary condition. The IDS for $H_{\omega,L}^{(D)}$ is

$$\mathcal{N}_{\omega,L}(E) = \frac{1}{2L+1} \times (\text{ number of eigenvalues} \leq E \text{ of } H_{\omega,L}^{(D)}) \tag{6.2}$$

For uniquely ergodic potentials $\mathcal{N}_{\omega,L}$ has an ω-independent limit, $\mathcal{N}(E)$, when L goes to infinity. As a limit of monotonically increasing functions, $\mathcal{N}(E)$ is monotonically increasing and can be shown to be continuous. It is, therefore, the distribution function of a continuous measure on $\mathbf{R}$, denoted also by $\mathcal{N}$. Furthermore, it can be shown that $\mathrm{supp}\,\mathcal{N} = \sigma(H)$. The use of Dirichlet boundary condition in the construction is not exclusive: any other boundary condition yielding a Hermitian restriction of $H(\omega)$ leads to the same IDS. (This, however, may not be true in higher dimensional spaces.) Obviously, the eigenvalues have to be counted with multiplicity.

The IDS for uniquely ergodic potentials can also be obtained by dealing directly with the infinite system. Fix any $V(\omega)$ and let $\mu_{\delta^n}(E)$, $n \in \mathbf{Z}$, be the distribution functions of the spectral measures for $H(\omega)$, associated with the canonical basis in $\ell^2(\mathbf{Z})$. Their average

$$\mathcal{N}_L(E) = \frac{1}{2L+1} \sum_{n=-L}^{L} \mu_{\delta^n}(E) \ ,$$

which is the distribution function of a measure ($\mathcal{N}_L$), converges to $\mathcal{N}(E)$ as L goes to infinity ([8]).

A part of the above results is easy to understand. If E is outside the spectrum, $f_0(\omega) = \mu_{\delta^0}(E)$ is a continuous function on the hull and, because of unique ergodicity, its average along trajectories exists and is independent of ω: this is $\mathcal{N}(E)$. If the spectrum is a Cantor set, the spectral gaps are dense everywhere (see Section 5.3) and $\mathcal{N}(E)$ has a unique extension from the gaps to $\mathbf{R}$ into an upper semicontinuous function. This, of course, does not explain, why is the spectrum a Cantor set and why is $\mathcal{N}(E)$ continuous. The IDS is constant in the gaps with values taken from a well-defined set (see Section 6.9).

Recall that the (pointwise) convergence of the distribution functions does not imply the convergence of the measures on *every* Borel set. For example, if $H(\omega)$ has a pure point spectrum, for each $E \in \sigma_{\mathrm{pp}}(H(\omega))$,

$$\mathcal{N}_L(\{E\}) \leq 1/(2L+1) \to 0 = \mathcal{N}(\{E\})$$

but $\mathcal{N}_L(\sigma_{\mathrm{pp}}(H(\omega))) = 1$ for each L while $\mathcal{N}(\sigma_{\mathrm{pp}}(H(\omega))) = 0$. In general, the infinite summation, which occurs because of the σ-additivity of $\mathcal{N}_L$, does not commute with the limit $L \to \infty$.

The above remark makes less surprising the observation, that the type of the measure $\mathcal{N}$ may have nothing to do with the type of the spectral measures. For example, in the case of random potentials, for ρ-a.e. ω the spectrum is pure point while $H(\omega)$ generates the same, continuous, IDS. In particular, $\mathcal{N}$ is absolutely continuous for smooth ρ. For Bernoulli distribution and sufficiently large potential strength $\mathcal{N}$ contains a singular continuous component with a support of positive Lebesgue measure ([28]). If the spectrum is a Cantor set of zero Lebesgue measure, a continuous $\mathcal{N}$ is necessarily singular continuous: examples are presented in Section 7. If the IDS is singular continuous, the *(differential) density of states* can be given no meaningful definition.

6.4   IDS and Lyapunov exponent

In Section 3.2 we introduced the Lyapunov exponent, more precisely, $\overline{\gamma}_{\pm}(E, V)$ and $\underline{\gamma}_{\pm}(E, V)$ for an arbitrary potential V. According to a theorem by Fürstenberg and Kesten [47], in the case of ergodic potentials there exists a function $\gamma(E)$ such that for every fixed E, for ρ-a.e. ω the four numbers coincide to give

$$\gamma(E, \omega) = \lim_{|n| \to \infty} \frac{1}{|n|} \ln \|T_{1 \to n}(E, \omega)\|$$

and $\gamma(E, \omega) = \gamma(E)$. A detailed study of many related questions, as, for example, the uniformicity in E of the convergence can be found in Goldsheid's work [53].

Let

$$
\begin{aligned}
S &= \{(E, \omega) : \ \gamma(E, \omega) \text{ does not exist or} \neq \gamma(E)\} \\
S_E &= \{\omega : (E, \omega) \in S\} \\
S^\omega &= \{E : (E, \omega) \in S\}
\end{aligned}
\tag{6.3}
$$

According to [47], for every E, $\rho(S_E) = 0$. By the Fubini theorem, $(m \times \rho)(S) = 0$ and, for ρ-a.e. ω, $m(S^\omega) = 0$.

In the theorem of Fürstenberg and Kesten the restriction to ρ-a.e. ω is essential, even if the potential is strictly ergodic. A counterexample is provided by the Almost-Mathieu equation for $\lambda > 2$ and α a Liouville number, where for any $E \in \sigma(H)$ the set S_E, defined above, is nonempty ([8]). However, for potentials generated by primitive substitutions, Hof [63] proved that S is empty.

There is a remarkable formula connecting the Lyapunov exponent to the IDS, found by Herbert and Jones [58] and Thouless [137]:

$$\gamma(E) = \int \ln |E - E'| \mathrm{d}\mathcal{N}(E') \tag{6.4}$$

The main observation leading to this formula is the following. For fixed ω let $H_{[1,L]}^{(D)}$ denote the restriction of $H(\omega)$ to the interval $[1, L]$ with Dirichlet boundary condition. It has an $L \times L$ matrix with $V(\omega)_1, ..., V(\omega)_L$ in the diagonal, 1 everywhere above and below the diagonal and 0 elsewhere. Let ψ be the solution of $H(\omega)\psi = E\psi$ with initial condition $\psi_0 = 0$, $\psi_1 = 1$. Then

$$\det(E - H_{[1,L]}^{(D)}) = \psi_{L+1}$$

Indeed, both members are polynomials of E of degree L, they have the same roots and the same principal coefficient. Let $E_{1,L}, ..., E_{L,L}$ be the roots, then

$$L^{-1}\ln|\psi_{L+1}(E)| = L^{-1}\sum_{i=1}^{L}\ln|E - E_{i,L}|$$

When $L \to \infty$, the two sides go to the respective sides of Eq.(6.4), apart from a set of (E, ω) of zero $m \times \rho$ measure. Equation (6.4) holds, in fact, for all $E \in \mathbf{C}$. The proof is based on the subharmonicity of $\gamma(E)$ and is due to Herman [59] and Craig and Simon [35].

6.5 Results on the set $\{E : \gamma(E) = 0\}$

Let us recall that for periodic potentials

$$\sigma(H) = \sigma_{\mathrm{ac}}(H) = G_0 \text{ where } G_0 = \{E : \gamma(E) = 0\}$$

For H_0, the pure kinetic energy operator, we still have $\sigma(H_0) = [-2, 2]$.

For almost periodic potentials Deift and Simon [38] found

$$m(G_0) \leq 4$$

with equality if and only if the potential is constant. In fact, this result extends to any ergodic potential (Last [92]).

Ishii [68] and Pastur [106] obtained the following result:
Let $V(\omega)$ be a bounded ergodic potential and P^ω denote the spectral resolution of the identity for $H(\omega)$. Suppose that $m(G_0) > 0$. Then for ρ-a.e. ω, P_{ac}^ω is concentrated on G_0.
The proof is easy: Choose a typical ω, such that $m(S^\omega) = 0$ (cf. Eq.(6.3)). The complement of G_0 can be written as $G_0^c = A \cup B$, where

$$A = \{E : \gamma(E, \omega) = \gamma(E) > 0\} \quad , \quad B = G_0^c \cap S^\omega$$

Now $P_{\mathrm{ac}}^\omega(B) = 0$ because P_{ac}^ω is absolutely continuous and B is of zero Lebesgue measure. On the other hand, for every $E \in A$, either there is no polynomially bounded solution or there is an exponentially localized solution. Therefore $P_{\mathrm{ac}}^\omega(A) = 0$ and, hence, $P_{\mathrm{ac}}^\omega(G_0^c) = 0$.

There is a different way to formulate this result. We can drop out of G_0 any set of zero Lebesgue measure and close the rest: P_{ac}^ω is still concentrated on this set which is now closed and, therefore, contains $\sigma_{\mathrm{ac}}(H(\omega))$. A particular closed set to which this remark applies is the essential closure of G_0.

The *essential closure* of a set A is

$$\overline{A}^{\,\mathrm{ess}} = \{E : m(A \cap (E - \varepsilon, E + \varepsilon)) > 0 \text{ for all } \varepsilon > 0\}$$

A short inspection may convince the reader that $\overline{A}^{\,\mathrm{ess}}$ is indeed a closed set, it is inside the closure of A, and what it does not contain from A is a set of zero Lebesgue measure:

$$m(A \setminus \overline{A}^{\,\mathrm{ess}}) = 0$$

Thus, the Ishii-Pastur theorem can be brought into the form

$$\sigma_{\mathrm{ac}}(H(\omega)) \subset \overline{G}_0^{\,\mathrm{ess}}$$

holding for ρ-a.e. ω.

What do we drop from G_0 when we take its essential closure? Imagine that, apart from an absolutely continuous spectrum, H has also a singular continuous spectrum on a disjoint set D of zero Lebesgue measure. If $\gamma(E) = 0$ on D, D belongs to G_0 but not to its essential closure. Similar is valid for a point spectrum on which the eigenvectors are not exponentially localized.

Most remarkably, the converse of the Ishii-Pastur theorem is also true and we have the following. For ρ-a.e. ω

$$\sigma_{\rm ac}(H(\omega)) = \overline{G}_0^{\,\rm ess} \tag{6.5}$$

Moreover, G_0 is an essential support for $P_{\rm ac}^\omega$.

This theorem was proven by Kotani for the differential equation ([86], [87]) and adapted by Simon to the difference equation ([129]).

Remarks.

(i) $\sigma_{\rm ac}(H(\omega))$ is the support of $P_{\rm ac}^\omega$, see Eq. (5.9), but it may not be an essential support. In fact, what we add to G_0 when taking its essential closure, may be a set of positive Lebesgue measure, see the example of Problem 5.6.3.

(ii) Since $\sigma_{\rm ac}(H(\omega)) \cap G_0$ is also an essential support for $P_{\rm ac}^\omega$, we have, in particular,

$$m(\sigma_{\rm ac}(H(\omega)) \cap G_0) = m(G_0)$$

for ρ-a.e. ω.

(iii) The main content of the above theorems is that the absolutely continuous spectrum of $H(\omega)$ is ρ-almost surely nonempty if and only if $m(G_0) > 0$. The 'if' is clear from the preceding remark; the 'only if' holds because $m(G_0) = 0$ implies that the essential closure of G_0 is empty.

6.6 The role of periodic approximants

Given a bounded aperiodic potential V, one can define a sequence of periodic approximants, V^k, in such a way that V^k converges to V pointwise. According to the second remark made in Section 6.2, $H^k = H_0 + V^k$ then tends strongly to $H = H_0 + V$ and Eq.(6.1) holds for the spectra. Our aim is to minimize the covering set on the left side of this equation, by choosing the best periodic approximants.

The best periodic approximants of potentials of the type $V(\omega)_n = g(n\alpha + \omega)$, where g is a period-1 function and α is irrational, are obtained by replacing α with its best rational approximants, α_k. For example, if $\alpha = (\sqrt{5} - 1)/2$, $\alpha_k = F_{k-1}/F_k$, where F_k is the kth Fibonacci number.

If V is a substitutional potential, V^k can be chosen to be the periodic repetition of the sequence $f(\omega_n)$, evaluated on the word $\eta^k(a)\eta^k(b)$ (cf. Sections 2 and 6.1).

6.7 Gordon-type theorems

Minimality sometimes implies that the potential repeats itself (exactly or with very good precision) on three neighboring intervals, one of which starting with 1, and this holds for an increasing sequence of interval lengths. In such cases, it can be shown that the Schrödinger equation has no solution decaying at the infinity, and thus the spectrum is purely continuous. The first proof of this kind was given by Gordon [54]. Suppose that

$$(V_{-L+1}...V_{-1}V_0) = (V_1...V_{L-1}V_L) = (V_{L+1}...V_{2L-1}V_{2L}) \tag{6.6}$$

Then

$$T_{-L+1 \to 0} = T_{1 \to L} = T_{L+1 \to 2L} = A_L$$

and, applying the two sides of the Caley-Hamilton equation

$$A_L^2 - (\operatorname{tr} A_L)A_L + I = 0 \tag{6.7}$$

to the vectors Ψ_{-L} and Ψ_0 (cf. Eq.(3.1)), one finds that for any solution ψ of the Schrödinger equation

$$\max\{\|\Psi_{-L}\|, \|\Psi_L\|, \|\Psi_{2L}\|\} \geq \frac{1}{2}\|\Psi_0\|$$

Clearly, if (6.6) holds for an increasing sequence L_n, no solution can decay on both sides, so there can be no eigenvector to H. Let us see two examples.

(i) Avron,Simon [8]: For the Almost-Mathieu equation, for $\lambda > 2$ and α Liouville number (for every positive integer k there are integers p_k and q_k such that $|\alpha - p_k/q_k| \leq k^{-q_k}$), for a.e. ω the spectrum is purely continuous. In this case, Eq.(6.6) does not hold exactly but with an extremely large precision. The spectrum is, in fact, purely singular continuous: this comes from the Ishii-Pastur-Kotani theorem, because $\gamma(E) > 0$ for all E ([4]).

(ii) Delyon, Petritis [43]: For circle potentials (see Section 2) with A being an interval, for every λ, a.e. ω and a.e. α the spectrum is purely continuous. In order that Eq.(6.6) hold true, some weak condition on the continued fraction expansion of α has to be imposed. This limits the result to almost every α.

A variant of the Gordon theorem uses only two intervals. Suppose that in Eq.(6.6) the second equality is verified for an increasing sequence L_n. This situation arises, for example, with substitutional potentials, if the substitutional sequence starts with a square. Applying the two sides of Eq.(6.7) to Ψ_0, one obtains

$$\max\{|\operatorname{tr} A_L| \|\Psi_L\|, \|\Psi_{2L}\|\} \geq \frac{1}{2}\|\Psi_0\|$$

This yields the absence of decaying solutions at $+\infty$ for energies such that

$$\operatorname{tr} T_{1 \to L_n}(E)$$

is a bounded sequence. In some cases one can show that this set of energies is just the spectrum (see [135] and Section 7).

6.8 Kotani theorem for potentials of finite range

Any periodic potential on $\ell^2(\mathbf{Z})$ is of finite range, i.e., takes on a finite number of different values. Any Schrödinger operator on $\ell^2(\mathbf{Z})$ with a periodic potential has a purely absolutely continuous spectrum. Therefore, the following theorem by Kotani [88] may be surprising. Let $V(\omega)$ be an ergodic nonperiodic finite-range potential, ρ the corresponding measure on the hull of V. Then, for ρ-a.e. ω, $H(\omega)$ has a purely singular spectrum.

This theorem is at the origin of many results on Schrödinger operators with circle- and substitutional potentials; we discuss them in the next section. It has long been an open question, whether the restriction to ρ-a.e. ω can be dropped, and whether the spectrum is purely singular continuous for every ω, if the potential is strictly ergodic. A recent result by Hof, Knill and Simon [64] goes in this direction: The authors show that for strictly ergodic potentials, either $H(\omega)$ has pure point spectrum for all ω or there is an uncountable dense set, although of zero ρ-measure, in the hull for which the spectrum is purely singular continuous. This latter case is shown to be realized for circle potentials if α is irrational and A is a half-open interval. This includes Sturmian potentials. Furthermore, for potentials generated by primitive substitutions, the Lyapunov exponent $\gamma(E, \omega)$ is independent of ω (Hof, [63]); Kotani's theorem then implies that the spectrum is purely singular for all ω.

6.9 Gap labeling

Gap labeling is a book-keeping for spectral gaps. The IDS naturally assigns a number to each gap: the (constant) value $\mathcal{N}(E)$ for E in the gap. The question is then to characterize this set of numbers. The first example of gap labeling for an almost periodic Schrödinger equation was given by Johnson and Moser [73] in the continuum case. The method used in the discrete case is quite different.

Problem 1. Let V be an L-periodic potential and suppose that $H = H_0 + V$ has no missing gap. Show that $\mathcal{N}(E) = k/L$, $k = 1, 2, ..., L-1$ in the gaps.

For strictly ergodic potentials, the values of the IDS in the gaps are taken from (but do not necessarily exhaust) a set S, determined by an algebraic theory, the K-theory. The application of K-theory to gap labeling was developed by Bellissard, Lima, Testard, Bovier and Ghez ([19], [16]). A detailed discussion can be found in [13], [14].

Sometimes it is possible to describe S quite explicitly. For example, according to Bellissard, Bovier and Ghez ([14], [13], [16], [27]), for circle and substitutional potentials S is the module (smallest additive group) containing the word frequencies of $V(\omega)$, restricted to the interval $[0, 1)$. This module contains the integers (the sum of the frequencies of cylinders with common base (n and k in Eq.(2.4)) is 1), therefore S is a group with respect to addition modulo 1, like for periodic potentials.

For Sturmian potentials this gives

$$S = \{k\alpha + m(1 - \alpha) : k, m \in \mathbf{Z}\} \cap [0, 1) = \{k\alpha + m : k, m \in \mathbf{Z}\} \cap [0, 1)$$

Notice that for $\alpha = K/L$, where K and L are relatively primes, this gives

$$S = \left\{ \frac{1}{L}, \frac{2}{L}, \ldots, \frac{L-1}{L} \right\} ,$$

in accordance with the assertion of the Problem above and the example (ii) in Section 4. If α is irrational, S is countably infinite and dense in $[0, 1]$. If there exist, indeed, gaps corresponding to values in a subset S' of S which is still dense in $[0, 1]$, the spectrum is necessarily a Cantor set and the IDS is continuous.

In our discussion of the periodic Schrödinger equation (Section 4) we introduced the notion of a missing gap (or closure of a gap). When there are no intervals in the spectrum, as is often the case with strictly ergodic potentials, what one can unambiguously assert is the *absence* of missing gaps or the *completeness of gap labeling*. Surely, there is no missing gap if

$$\operatorname{Ran}_g \mathcal{N} \equiv \{\mathcal{N}(E): \ E \text{ is in a spectral gap}\} = S , \tag{6.8}$$

the set of all the admissible values. (Notice that each admissible value is taken on in at most a single gap.) As in the periodic case, there is no general method to check whether or not all the gaps open. This is known to hold true in a few cases, like the period doubling potential or the Fibonacci potential with $\lambda > 4$.

Example. For the classical Cantor set, in the kth gap on the nth level ($n = 0, 1, ...; \ k = 1, ..., 2^n$) the Cantor function $\alpha(x) = (2k - 1)/2^{n+1}$. These numbers form an additive group modulo 1. The same values are taken by the IDS of the hierarchical Hamiltonian ([90], see also [89]) in the domain of the parameters where the potential is limit periodic. In this case the gap labeling is complete.

7 Schrödinger equation with Sturmian and substitutional potentials

7.1 Fibonacci potential

Fibonacci substitution was the first to be used to define a two-valued potential (see Section 2) and to study the spectral problem of the corresponding Schrödinger operator (Kohmoto, Kadanoff and Tang, Ostlund et al. [79], [80], [81], Casdagli [30], Sütő [135], [136]). This is also the first example where the trace map ([2], [84], [111]) was fully exploited.

The Fibonacci sequence, as any minimal sequence, has almost-periods: these are the Fibonacci numbers F_n ($F_0 = F_1 = 1, F_{n+1} = F_n + F_{n-1}$). Choose, for example,

$$V_n = \lambda(\lfloor (n+1)\alpha \rfloor - \lfloor n\alpha \rfloor) \tag{7.1}$$

then the almost-periodicity is expressed by the equations

$$
\begin{aligned}
V_{l+F_n} &= V_l \ \text{ if } n \geq 3 \text{ and } 1 \leq l \leq F_n \\
V_{l-F_{2n}} &= V_l \ \text{ if } n \geq 1 \text{ and } 1 \leq l \leq F_{2n+1}
\end{aligned}
$$

The transfer matrices over the almost-periods replace the single transfer matrix $T_{1 \to L}$ in the L-periodic case. For an L-periodic potential

$$T_{1 \to 2L} = T_{1 \to L}^2 \tag{7.2}$$

Let
$$M_n = T_{1 \to F_n}$$
For the Fibonacci potential Eq.(7.2) is replaced by
$$M_{n+1} = M_{n-1}M_n$$
This, together with $\det M_n = 1$, implies for $\tau_n = \operatorname{tr} M_n$ the recurrence relation
$$\tau_{n+2} = \tau_{n+1}\tau_n - \tau_{n-1}$$
The initial conditions (with the choice (7.1))
$$\tau_{-1} = 2 \ , \ \tau_0 = E \ , \ \tau_1 = E - \lambda$$
contain only 2 parameters, and this indicates that the recurrence must have a nontrivial invariant. Indeed,
$$\tau_{n+1}^2 + \tau_n^2 + \tau_{n-1}^2 - \tau_{n+1}\tau_n\tau_{n-1} - 4 = (\tau_1 - \tau_0)^2 = \lambda^2$$
From the trace map and the invariant, the following results can be deduced ([135], [136]).

1. $\sigma(H) = \{E : \{\tau_n(E)\}_{n=1}^\infty$ is bounded$\}$
   (Remember that for an L-periodic potential $\sigma(H) = \{E : |\operatorname{tr} T_{1 \to L}(E)| \leq 2\}$.)

2. The spectrum of $H(\omega = 0)$ is purely continuous (the proof is of Gordon-type with two intervals).

3. $\gamma(E, \omega = 0) = 0$ for all $E \in \sigma(H)$.

4. The Lebesgue measure $m(\sigma(H)) = 0$ (found by confronting the Ishii-Pastur-Kotani theorem with Kotani's theorem for potentials of finite range). As a consequence, $\sigma(H)$ is a Cantor set (because $\sigma(H)$ contains no isolated point).

5. The spectrum of $H(\omega = 0)$ is purely singular continuous.

6. For all $E \in \sigma(H)$ all solutions of $H(\omega = 0)\psi = E\psi$ are polynomially bounded (Iochum, Raymond, Testard [66], [67]).

It is an open question whether the spectrum is purely singular continuous for all ω. Let us recall that $TH(\omega)T^{-1} = H(T\omega) = H(\omega + \alpha)$ is unitary equivalent to $H(\omega)$, therefore the singular continuity holds true for $\omega = k\alpha \pmod 1$, $k \in \mathbf{Z}$, which is a countable dense set in $[0, 1]$. Due to [64], this result has recently been extended to an uncountable dense set of ω, still of zero measure (cf. Section 6.8).

7.2   General Sturmian potentials

The case of Sturmian potentials for arbitrary irrational α was investigated by Bellissard, Iochum, Scoppola and Testard [17]. The methods applied to the Fibonacci case can be extended to treat the general problem, even though this is technically more involved. All the results found for the Fibonacci potential remain valid and the same questions are unanswered.

There is an interesting numerical work by Ostlund and Kim [OK] and a rigorous study by Bellissard, Iochum and Testard [18] on the α-dependence of the spectrum of $H = H_0 + V^{(\alpha)}$, where
$$V_n^{(\alpha)} = X_{[0,\alpha)}(n\alpha) \ ,$$
cf. Section 2. For rational α the potential is periodic and the spectrum is the union of a finite number of intervals. When approaching a rational α from above and from below, the numerical plot of the energies belonging to the spectrum clearly reveals a discontinuity, see Figure 2. [18] show that this reflects the discontinuity of the characteristic function which generates the potential. The gap edges vary continuously on irrational α's. For a rational value r,
$$\lim_{\alpha \uparrow r} V^{(\alpha)} \neq \lim_{\alpha \downarrow r} V^{(\alpha)}$$

and none of them equals $V^{(r)}$. In fact, the two limits are not periodic, only ultimately periodic (as if we took a periodic sequence, cut off a finite segment which is not a period and glue the two infinite pieces together). Both yield the same essential spectrum as $H_0 + V^{(r)}$ and both create (different) isolated eigenvalues in the gaps.

7.3   Period doubling potential

The potential is generated by the period doubling substitution $\xi(a) = ab$, $\xi(b) = aa$. The corresponding Schrödinger equation was studied by Bellissard, Bovier and Ghez [15], [27]. The trace map is a fundamental tool of the analysis. Results 1.-5. valid for the Fibonacci potential hold true: The spectrum is a Cantor set of zero Lebesgue measure, it is purely singular continuous (again, not known for all elements of the hull) and the Lyapunov exponent vanishes in the spectrum. There is a rather detailed knowledge about the gaps, their behavior as a function of the potential strength. Gap labeling is complete: all admissible values are taken by the IDS in the gaps.

7.4   Thue-Morse potential

Historically, the first studies were done by Axel et al. on the phonon frequency spectrum of the harmonic chain with masses generated by the Thue-Morse substitution $\xi(a) = ab$, $\xi(b) = ba$. In [9], [10], [11] we find the proof that the phonon spectrum is a Cantor set, a numerical work on its box dimension suggesting zero Lebesgue measure, gap labeling and a study of generalized eigenfunctions. This latter established the existence of extended states for a dense set in the phonon spectrum.

The Schrödinger equation with the potential generated by this substitution has also been widely studied, namely by Bellissard [12], Delyon and Peyrière [43] and Bovier and Ghez [26], [27]. Valuable numerical work was done by Riklund et al. [121]. Bellissard [12] identified the set $\text{Ran}_g \mathcal{N}$ (cf. (6.8)) and studied the dependence of the gap widths on the potential strength. Delyon and Peyrière [43] proved the absence of decaying solutions and, hence, the continuity of the spectrum. They showed that the generalized eigenfunctions are not 'too small' on a geometric progression. The continuity of the spectrum was obtained as a byproduct also in [15], [27]. Bovier and Ghez [26], [27] proved, in a more general context (see next section), that the spectrum is of zero Lebesgue measure. With the continuity this implies that the spectrum is purely singular continuous.

7.5   Systematic study of substitutional potentials

Bovier and Ghez [26], [27] succeeded to find a general condition on primitive substitutions, assuring that the corresponding Schrödinger operator has a spectrum of zero Lebesgue measure. Their work deeply exploits the Kolár-Nori results on trace maps ([84], see also [111]).

The action of a substitution ξ can be defined on transfer matrices and on traces of transfer matrices. ξ acting on traces is called a *trace map*. ξ carries a letter a of the alphabet $\mathcal{A}$ into a word, the transfer matrix corresponding to a into a product, i.e. a *monomial*, of transfer matrices in reversed order, and the trace of the transfer matrix into a *polynomial* of traces of transfer matrices belonging to letters of an enlarged alphabet $\mathcal{B}$. These generalized letters are special words over the original alphabet $\mathcal{A}$, not containing repeated letters of $\mathcal{A}$. Therefore $\mathcal{B}$ is also finite, and one can see that the trace map is closed in the following sense:
ξ carries the trace belonging to any letter of $\mathcal{B}$ into a polynomial of traces belonging to letters of $\mathcal{B}$.

Let $b_1, ..., b_q$ be the letters of $\mathcal{B}$ and x_i a real variable associated with b_i. The idea of Bovier and Ghez is to retain the highest degree monomial

$$\tilde{f}_i(x_1, ... x_q) = \prod_{j=1}^{q} x_j^{k_{ij}}$$

of the polynomial corresponding to b_i and to define a substitution ϕ on $\mathcal{B}$ such that $\phi(b_i)$ contains b_j k_{ij} times. Based on earlier experience, namely with the Fibonacci substitution, one may expect that, by imposing some conditions on ϕ, it is possible to control the high iterates of the trace map

and, hopefully, the spectrum. The right notion is *semi-primitivity*, a property which is somewhat weaker than primitivity (see [26] for the definition) and is straightforward to verify. The authors prove that, if ξ is primitive, ϕ is semi-primitive and the substitutional sequence contains the word bb for some $b \in \mathcal{B}$, $\sigma(H)$ is a set of zero Lebesgue measure. Although the proof is more complicated than in the cases discussed earlier, the main idea is again to show that the Lyapunov exponent vanishes in the spectrum (the existence of the word bb is used here) and, then, to confront the Ishii-Pastur-Kotani theorem with the Kotani theorem for finite-ranged potentials. If the substitutional sequence starts with a square, the two-interval version of the Gordon theorem yields also that the spectrum is purely singular continuous.

The conditions of the theorem are fulfilled by many named substitutional sequences as, for example, the Fibonacci, Thue-Morse, period doubling, binary non-Pisot, ternary non-Pisot and circle sequences. Apart from the binary non-Pisot sequence, singular continuity is also verified in the cases listed above (but it is not proved for the other potentials in the hull). A notable exception is the Rudin-Shapiro substitution which is primitive and therefore the spectrum is purely singular ([64]), but for which the substitution ϕ is not semi-primitive and, hence, it is not known whether $\sigma(H)$ is of zero Lebesgue measure.

8 Solutions to the problems

2.1

The proof is based on the observation that for bounded sequences pointwise convergence is equivalent to convergence in the metric d.

(i) 1. implies 2.

Indeed, $s \in \Omega(s) = \Omega(t)$.

(ii) 2. implies 3.

$\Omega(s)$ is bounded: for all $t \in \Omega(s)$, $d(s, t) \leq 6 \sup |s_n|$.

Suppose that s is not almost-periodic. Then there exists an $\varepsilon > 0$ and an infinite sequence of real intervals (a_k, b_k) such that $b_k - a_k \to \infty$ and $d(T^n s, s) > \varepsilon$ for every integer $n \in \cup(a_k, b_k)$. Choose an integer n_k in (a_k, b_k) such that $n_k - a_k \to \infty$ and $b_k - n_k \to \infty$. Since $\Omega(s)$ is closed and bounded (compact in the topology generated by d), $T^{n_k} s$ has at least one limit point t in $\Omega(s)$. Fix an arbitrary integer n. We have the triangle inequality

$$d(s, T^n t) \geq d(s, T^{n_k+n} s) - d(T^{n_k+n} s, T^n t) .$$

For k sufficiently large, $n_k + n \in (a_k, b_k)$ and thus $d(s, T^{n_k+n} s) > \varepsilon$. On the other hand, $d(T^{n_k} s, t) \to 0$ implies that $d(T^{n_k+n} s, T^n t) \to 0$ as $k \to \infty$. It follows that $d(s, T^n t) \geq \varepsilon$ for all integers n. Hence, s cannot be in $\Omega(t)$, which contradicts 2.

(iii) 3. implies 2.

Let $t \in \Omega(s)$, $t = \lim_{j \to \infty} T^{i_j} s$, where lim means pointwise limit. Fix an $\varepsilon > 0$ and let $\{n_k\}$ be the almost-periods with gaps smaller than ℓ_ε. Given j, choose k such that $n_{k-1} < i_j < n_k$. Then $m_j \equiv n_k - i_j < \ell_\varepsilon$ and

$$
\begin{aligned}
d(s, T^{m_j} t) &\leq d(s, T^{n_k} s) + d(T^{n_k} s, T^{m_j} t) \\
&\leq \varepsilon + d(T^{m_j} T^{i_j} s, T^{m_j} t)
\end{aligned}
$$

Take the limit $j \to \infty$. Since $0 < m_j < \ell_\varepsilon$, there will be an $m \in (0, \ell_\varepsilon)$ which occurs infinitely many times among the m_j's. Taking the limit only on the subsequence of j values for which $m_j = m$, we obtain $d(s, T^m t) \leq \varepsilon$. Since ε was arbitrary, this proves that $s \in \Omega(t)$.

(iv) 2. implies 1.

Suppose $t \in \Omega(s)$. Then $T^n t \in \Omega(s)$ for every integer n, because $\Omega(s)$ is shift-invariant. $\Omega(s)$ being closed, this implies $\Omega(t) \subset \Omega(s)$. On the other hand, according to 2., $s \in \Omega(t)$. Interchanging s and t, the above argument yields $\Omega(s) \subset \Omega(t)$.

2.2

Let $A \subset \Omega(s)$ be a T-invariant set. One has to show that $\rho(A) = 0$ or 1. Suppose the opposite, i.e., $0 < \rho(A) < 1$. Define a probability measure μ by setting

$$\mu(B) = \rho(A \cap B)/\rho(A)$$

It is easy to verify that μ is a T-invariant probability; on the other hand, it differs from ρ (e.g., on $\Omega(s) \setminus A$). This contradicts the uniqueness of ρ.

2.3

Let $\omega \in \Omega$. If $\{T^n \omega\}_{n=0}^{\infty}$ is an infinite set, the sequence contains no repetition. Therefore

$$1 \geq \rho(\{T^n \omega\}_{n=0}^{\infty}) = \sum_{n=0}^{\infty} \rho(\{T^n \omega\}) = \sum_{n=0}^{\infty} \rho(\{\omega\})$$

and hence $\rho(\{\omega\}) = 0$.

3.2.1

The proof goes by induction. $\operatorname{tr} A^0 = \operatorname{tr} I = 2$. Multiplying the Caley-Hamilton equation

$$A^2 - (\operatorname{tr} A)A + I = 0$$

with A^{k-2} and taking the trace one finds

$$\operatorname{tr} A^k = \operatorname{tr} A \operatorname{tr} A^{k-1} - \operatorname{tr} A^{k-2}$$

in which one may recognize the recurrence relation for the Chebyshev polynomials. Setting $\operatorname{tr} A = 2 \cos \alpha$, the solution of the recurrence is

$$\operatorname{tr} A^k = 2 \cos k\alpha$$

.

5.1.1

Let $H\psi = E\psi$ where ψ is subexponential: for any $a > 0$ there exists a $b > 0$ such that

$$|\psi_k| < be^{a|k|} \quad \text{for all } k,$$

but ψ is not in $\ell^2(\mathbf{Z})$. It follows that either $\sum_{k=0}^{\infty} |\psi_k|^2 = \infty$ or $\sum_{k=-\infty}^{0} |\psi_k|^2 = \infty$. Suppose, for instance, the first. Define $\psi^n = \psi/(\sum_{l=0}^{n} |\psi_l|^2)^{1/2}$ for $n > 0$. Then $H\psi^n = E\psi^n$, and φ^n, given by

$$\varphi_k^n = \begin{cases} \psi_k^n & \text{if } 0 \leq k \leq n \\ 0 & \text{otherwise} \end{cases}$$

is a normalized vector for all n. We show that a suitable subsequence of $\{\varphi^n\}_{n=1}^{\infty}$ is a Weyl sequence. It is clear that for all k, $\varphi_k^n \to 0$ with increasing n, so φ^n goes to zero weakly. On the other hand,

$$(H\varphi^n)_k = E\varphi_k^n \quad \text{if } k \neq -1, 0, n, n+1$$

This implies that

$$\varepsilon_k^n = 0 \quad \text{if } k \neq -1, 0, n, n+1$$

(cf. Eq.(5.3)). It is easy to check that

$$\varepsilon_{-1}^n = \psi_0^n \quad \varepsilon_0^n = -\psi_{-1}^n \quad \varepsilon_n^n = -\psi_{n+1}^n \quad \varepsilon_{n+1}^n = \psi_n^n$$

Therefore

$$\|\varepsilon^n\|_{\ell^2}^2 = \|\Psi_{-1}^n\|^2 + \|\Psi_n^n\|^2$$

where the vectors on the right correspond to the definition (3.1). The first term goes to zero as n increases, the second, in general, not. However, there exists a subsequence n_k such that $\|\Psi_{n_k}^{n_k}\| \to 0$ with increasing k. Indeed, if the opposite were true, one could find a positive constant c such that $\|\Psi_n^n\|^2 > c$ for all $n > 0$. Now

$$c < \|\Psi_n^n\|^2 = \|\Psi_n\|^2 / \sum_{k=0}^{n} |\psi_k|^2 \leq 2\|\Psi_n\|^2 / \sum_{k=0}^{n-1} \|\Psi_k\|^2$$

and therefore

$$\|\Psi_n\|^2 > \frac{c}{2}\sum_{k=0}^{n-1}\|\Psi_k\|^2 > \frac{c}{2}(\frac{c}{2}+1)\sum_{k=0}^{n-2}\|\Psi_k\|^2 > \cdots > \frac{c}{2}(\frac{c}{2}+1)^{n-1}\|\Psi_0\|^2$$

which contradicts the supposed subexponential nature of ψ. The Weyl sequence we were looking for is $\{\varphi^{n_k}\}_{k=1}^{\infty}$.

5.2.1

In general, let E be any accumulation point of the eigenvalues of H, say, $E_n \to E$ as $n \to \infty$. Let ψ^n be the corresponding orthonormal eigenvectors. Then ψ^n form a Weyl sequence. First, they go to zero weakly: for any vector $\varphi \in \mathcal{H}$, the Bessel inequality

$$\|\varphi\|^2 \geq \sum_{n=1}^{\infty}|(\psi^n, \varphi)|^2$$

implies that $(\psi^n, \varphi) \to 0$ with increasing n. Second,

$$H\psi^n = E_n\psi^n = E\psi^n + (E_n - E)\psi^n$$

and $\|(E_n - E)\psi^n\| = |E_n - E| \to 0$.

5.2.2

Choose a sequence n_k such that $V_{n_k} \to E$ as $k \to \infty$. If δ^n is the unit vector concentrated on n,

$$\|(E - V)^{-1}\delta^{n_k}\| = 1/|E - V_{n_k}| \to \infty ,$$

so the inverse of $E - V$ is unbounded. By definition, this means that E is in the spectrum.

One can also construct a vector ψ such that the solution of $(E - V)\varphi = \psi$ for φ, given by

$$\varphi_n = \psi_n/(E - V_n) ,$$

is not square-summable. Write $E = \cos 2\pi\theta$, then trivially

$$|E - V_n| \leq 2\pi \min_{p\in\mathbf{Z}}|n\alpha - \theta - p|$$

On the other hand, by the Kronecker theorem (Theorem 440 in [57]), there exists an increasing sequence n_k of positive integers and a sequence p_k of integers such that

$$|n_k\alpha - \theta - p_k| < 3/n_k$$

The example is obtained by choosing $\psi_n = E - V_n$ for $n = n_k$ and zero otherwise: $\|\psi\|^2 < 6\pi^4$ but $\varphi_{n_k} = 1$ for all k, so φ is not square-summable.

5.6.1

If x is not in supp μ then for sufficiently small $\varepsilon > 0$, $\mu(x+\varepsilon) - \mu(x-\varepsilon) = \mu((x-\varepsilon, x+\varepsilon)) = 0$ and, hence, x is not a point of increase of the distribution function. If $x \in$ supp μ then for every $\varepsilon > 0$,
$$\mu(x + \varepsilon) - \mu(x - \varepsilon) = \mu((x - \varepsilon, x + \varepsilon]) \geq \mu((x - \varepsilon, x + \varepsilon)) > 0 ,$$
that is, x is a point of increase.

5.6.2

Let μ, ν be ac measures, A a common essential support. Suppose that $\mu(B) = 0$. $\nu(B\cap A^c) = 0$ because A is an essential support of ν. $m(B \cap A) = 0$, because $B \cap A \subset A$, an essential support of μ, and $\mu(B \cap A) = 0$. But ν is ac, so $\nu(B \cap A) = 0$. We found $\nu \ll \mu$. The opposite is obtained by interchanging μ and ν.

5.6.3

(i) Let C be a 'thick' Cantor set (i.e., $m(C) > 0$),

$$C^c = \cup_{n=0}^{\infty}C_n^c = \cup_{n=0}^{\infty}\cup_{k=1}^{k_n} J_{nk}$$

where J_{nk} are the open intervals appearing in the construction of C (cf. Sec.5.3). Let $f_{nk}(x)$ be a continuous function which is strictly positive on J_{nk} and vanishes outside J_{nk}, and

$$\sum_{n=0}^{\infty} \sum_{k=1}^{k_n} \int f_{nk}(x) \mathrm{d}x < \infty$$

Then $\sum_n \sum_k f_{nk}$ is the density of an absolutely continuous measure μ. $\operatorname{supp}\mu = \mathbf{R}$ (because the closure of C^c is $\mathbf{R}$), and an essential support of μ is C^c. So $\mu(C) = 0$ but $m(C) > 0$, therefore $\operatorname{supp}\mu$ is not an essential support of μ.

(ii) For $0 < p < q$, p and q integers which are relatively primes, let $\mu(\{p/q\}) = 2^{-p-q}$. $\operatorname{supp}\mu = [0,1]$ while the rational numbers in $(0,1)$ form an essential support. $\mu([0,1] \setminus \mathbf{Q}) = 0$ but $m([0,1] \setminus \mathbf{Q}) = 1$, so the support is not an essential support.

(iii) Let μ be concentrated on a discrete set (whose only accumulation points can be $\pm\infty$), for instance, $\mu(\mathbf{R}) = \sum_{n=1}^{\infty} \mu(\{n\})$. Then $\operatorname{supp}\mu$ is the smallest essential support.

5.6.4

(i) If $\mu(x)$ is absolutely continuous (ac) on any finite interval then the measure μ is ac.
Indeed, let A be a Borel set, $m(A) = 0$ and suppose first that A is covered by a finite open interval J. Fix $\varepsilon > 0$ and let $\delta > 0$ correspond to ε (cf. Eq.(5.7)). According to the definition of a set of zero Lebesgue measure, one can find an open set O such that $A \subset O$ and $m(O) < \delta$. O is the union of disjoint open intervals $(a_1, b_1), (a_2, b_2), ...$, all in J, so that $A \subset \cup(a_i, b_i)$ and $\sum(b_i - a_i) < \delta$. Thus,

$$\mu(A) < \sum \mu((a_i, b_i)) = \sum (\mu(b_i) - \mu(a_i)) < \varepsilon$$

Since ε is arbitrary, $\mu(A) = 0$.

If A is not covered by a finite interval, it is covered by countably many finite intervals J_k. $\mu(A \cap J_k) = 0$ for all k, thus $\mu(A) = 0$.

(ii) If μ is an ac measure, i.e., $\mu \ll m$, then $\mu(x)$ is an ac function on any finite interval.
We show this by proving that, given a finite interval J, for any $\varepsilon > 0$ there exists a $\delta > 0$ such that for Borel sets $A \subset J$, $m(A) < \delta$ implies $\mu(A) < \varepsilon$. Suppose this does not hold true. Then there exists an $\varepsilon > 0$ such that for all $n \geq 1$ and for suitably chosen $A_n \subset J$, $m(A_n) < 1/2^n$ but $\mu(A_n) \geq \varepsilon$. Let $B_n = \cup_{k=n+1}^{\infty} A_k$. Now $m(B_n) \leq 1/2^n$ and $\mu(B_n) \geq \mu(A_{n+1}) \geq \varepsilon$. Since $B_n \subset J$ for all n and B_n is a decreasing sequence, it has a limit $B \subset J$ for which $m(B) = 0$ and $\mu(B) \geq \epsilon$. This contradicts $\mu \ll m$.

5.6.5

Suppose μ is a singular measure. Then there is some set A of zero Lebesgue measure such that μ is concentrated on A. The intersection of any essential support with A yields an essential support of zero Lebesgue measure. If B is an essential support and $m(B) > 0$ then $\mu(B \setminus A) = 0$ and $m(B \setminus A) > 0$, a contradiction.

5.6.6

The definition of μ_{pp} is constructive, see Eq.(5.6), therefore the pp part is unique. Let

$$\mu = \mu_{\mathrm{pp}} + \mu_{\mathrm{sc}}^1 + \mu_{\mathrm{ac}}^1 = \mu_{\mathrm{pp}} + \mu_{\mathrm{sc}}^2 + \mu_{\mathrm{ac}}^2$$

If $\mu_{\mathrm{sc}}^1 \neq \mu_{\mathrm{sc}}^2$, there exists a set Δ such that $m(\Delta) = 0$ and $\mu_{\mathrm{sc}}^1(\Delta) \neq \mu_{\mathrm{sc}}^2(\Delta)$. But then $\mu_{\mathrm{ac}}^1(\Delta) \neq \mu_{\mathrm{ac}}^2(\Delta)$ which contradicts $\mu_{\mathrm{ac}}^1(\Delta) = \mu_{\mathrm{ac}}^2(\Delta) = 0$.

5.7.1

Let C be the middle-thirds Cantor set, α the sc measure whose distribution function is the Cantor function. Let μ be a pp measure whose smallest essential support is the set of boundary points $\{c_{ni}\}$ of the complement of C, cf. Sec. 5.3. Then $\operatorname{supp}\mu = \operatorname{supp}\alpha = C$ and C is also an essential support for both measures.

5.8.1

The following statements are equivalent: μ_ψ is concentrated on A, $\mu_\psi(\mathbf{R}) = \mu_\psi(A)$, $\|\psi\|^2 = \|P(A)\psi\|^2$, $\|(I - P(A))\psi\| = 0$, $(I - P(A))\psi = 0$, $P(A)\psi = \psi$.
If $\psi \in P(A)\mathcal{H}$ then $P(A)\psi = \psi$, so $\mu_\psi(A^c) = 0$ and $\operatorname{supp}\mu_\psi \subset \overline{A}$.

5.8.2

Let A be any Borel set such that μ_ψ is concentrated on A. Then from Problem 5.8.1, $P(A)\psi = \psi$. H commutes with $P(A)$, therefore $P(A)H\psi = H\psi$. From Problem 5.8.1 it follows that $\mu_{H\psi}$ is concentrated on A. By definition, we get $\mu_{H\psi} \ll \mu_\psi$.

If μ_ψ is singular, it is concentrated on a set A such that $m(A) = 0$. Therefore $\mu_{H\psi}$ is also singular. If μ_ψ is continuous, for any $E \in \mathbf{R}$, $\mu_\psi(\{E\}) = \|P(\{E\})\psi\|^2 = 0$, therefore $P(\{E\})\psi = 0$. Hence,

$$\mu_{H\psi}(\{E\}) = \|P(\{E\})H\psi\|^2 = \|HP(\{E\})\psi\|^2 = 0 ,$$

that is, $\mu_{H\psi}$ is continuous. So $\mu_{H\psi}$ is sc if μ_ψ is sc. If μ_ψ is ac then $\mu_{H\psi}$ is ac because $m(A) = 0$ implies $\mu_\psi(A) = 0$, which implies $\mu_{H\psi}(A) = 0$.

5.8.3

Let A, B, C be disjoint essential supports respectively for $(\mu_\psi)_{\mathrm{pp}}, (\mu_\psi)_{\mathrm{ac}}, (\mu_\psi)_{\mathrm{sc}}$. μ_ψ is concentrated on $A \cup B \cup C$. From Problem 5.8.1,

$$\psi = P(A \cup B \cup C)\psi = P(A)\psi + P(B)\psi + P(C)\psi \equiv \psi^{\mathrm{pp}} + \psi^{\mathrm{ac}} + \psi^{\mathrm{sc}}$$

Now

$$P(A)P(B) = P(A)P(C) = P(B)P(C) = 0$$

therefore $\psi^{\mathrm{pp}}, \psi^{\mathrm{ac}}, \psi^{\mathrm{sc}}$ are pairwise orthogonal, and for any Borel set Δ

$$\begin{aligned}
\mu_\psi(\Delta) = \|P(\Delta)\psi\|^2 &= \|P(\Delta)P(A)\psi\|^2 + \|P(\Delta)P(B)\psi\|^2 + \|P(\Delta)P(C)\psi\|^2 \\
&= \mu_{\psi^{\mathrm{pp}}}(\Delta) + \mu_{\psi^{\mathrm{ac}}}(\Delta) + \mu_{\psi^{\mathrm{sc}}}(\Delta)
\end{aligned}$$

Using the relations $P(\Delta)P(A) = P(\Delta \cap A)$, etc., we find

$$\mu_{\psi^{\mathrm{pp}}}(\Delta) = \mu_\psi(\Delta \cap A) = (\mu_\psi)_{\mathrm{pp}}(\Delta)$$

and so on.

5.8.4

(i) Let B be any Borel set, then

$$\begin{aligned}
\mu_{\psi^i}(B) = \|P(B)\psi^i\|^2 &= (\psi, P(B)\psi) + (\psi^i - \psi, P(B)\psi^i) + (\psi, P(B)(\psi^i - \psi)) \\
&= \mu_\psi(B) + O(\|\psi^i - \psi\|) \to \mu_\psi(B)
\end{aligned}$$

(ii) ψ^i are singular, so there exist sets A_i such that $\mu_{\psi^i}(A_i^c) = 0$ and $m(A_i) = 0$. Now $m(\cup A_i) = 0$, for all i $\mu_{\psi^i}((\cup A_j)^c) \le \mu_{\psi^i}(A_i^c) = 0$ and by (i), $\mu_\psi((\cup A_j)^c) = 0$. So μ_ψ is concentrated on a set of zero Lebesgue measure and, hence, is singular. If all the μ_{ψ^i} are pp or all are sc then μ_ψ is pp or sc, respectively, because $\mathcal{H}_{\mathrm{pp}}$ and $\mathcal{H}_{\mathrm{cont}}$ are closed subspaces.

5.8.5

(i) $[\mathcal{H}_{\mathrm{ac}}]P$ is ac: Let B be a Borel set, $m(B) = 0$. Take any $\psi \in \mathcal{H}$, then

$$\|[\mathcal{H}_{\mathrm{ac}}]P(B)\psi\|^2 = \|P(B)[\mathcal{H}_{\mathrm{ac}}]\psi\|^2 = \mu_{\psi^{\mathrm{ac}}}(B) = (\mu_\psi)_{\mathrm{ac}}(B) = 0$$

therefore $[\mathcal{H}_{\mathrm{ac}}]P(B) = 0$.

(ii) $[\mathcal{H}_{\mathrm{sc}}]P \le [\mathcal{H}_{\mathrm{cont}}]P = P_{\mathrm{cont}}$, therefore $[\mathcal{H}_{\mathrm{sc}}]P$ is a continuous measure. We have to prove that it is singular. Choose an orthonormal basis $\{\psi_i\}$. Let A_i be sets of zero Lebesgue measure, $\mu_{\psi_i^{\mathrm{sc}}}$ concentrated on A_i. Take $A = \cup A_i$. $m(A) = 0$ and we show that $[\mathcal{H}_{\mathrm{sc}}]P$ is concentrated on A.

$$\|P(A^c)[\mathcal{H}_{\mathrm{sc}}]\psi_i\| = \|P(A^c)\psi_i^{\mathrm{sc}}\| = \|P(\cap_j A_j^c)\psi_i^{\mathrm{sc}}\| = \|\prod_{j \ne i} P(A_j^c)P(A_i^c)\psi_i^{\mathrm{sc}}\| = 0$$

The last equality holds because $P(A_i^c)\psi_i^{\mathrm{sc}} = 0$, according to Problem 5.8.1. It follows that $[\mathcal{H}_{\mathrm{sc}}]P(A^c)\psi_i = 0$ for all i, and therefore $[\mathcal{H}_{\mathrm{sc}}]P(A^c) = 0$.

5.8.6

If $\mu(B) = 0$ then $\mu_\psi(B) = 0$ for all $\psi \in \mathcal{H}$. Accordingly, $\|P(B)\psi\| = 0$ for all $\psi \in \mathcal{H}$ which means that $P(B) = 0$.

5.8.7

Let B be a Borel set, $\mu_{\psi^1}(B) + \mu_{\psi^2}(B) = 0$. Then $\|P(B)\psi^1\| = \|P(B)\psi^2\| = 0$ and hence $P(B)\psi^1 = P(B)\psi^2 = 0$. This implies

$$
\begin{aligned}
\mu_{\alpha\psi^1+\beta\psi^2}(B) &= |\alpha|^2\|P(B)\psi^1\|^2 + |\beta|^2\|P(B)\psi^2\|^2 \\
&+ \alpha^*\beta(\psi^1, P(B)\psi^2) + \alpha\beta^*(\psi^2, P(B)\psi^1) = 0
\end{aligned}
$$

5.8.8

According to Problem 5.8.6, it suffices to show that $\mu_\psi \ll \sum c_i \mu_{\psi^i}$ for all $\psi \in \mathcal{H}$. Writing $\psi = \sum \alpha_i \psi^i$, one proves

$$
\mu_{\Sigma\alpha_i\psi^i} \ll \sum c_i \mu_{\psi^i}
$$

exactly as in Problem 5.8.7.

5.8.9

(i) The set is linearly independent: Taking any finite linear combination with not all coefficients vanishing and expanding the sum in the canonical basis $\{\delta^n\}$, at least one δ^n appears with nonzero coefficient.

(ii) The set generates the canonical basis $\{\delta^n\}_{n=-\infty}^{\infty}$. For $n = 0$ one obtains δ^0, δ^1 and by induction one finds that $\delta^{-n}, \delta^{-n+1}, ..., \delta^n, \delta^{n+1}$ can be expanded with the vectors $\{H^k\delta^0, H^k\delta^1\}_{k=0}^n$.

5.8.10

Let $\psi^1 \in \mathcal{H}_1$ and $\psi^2 \in \mathcal{H}_2$ where $\mathcal{H}_i$ are subspaces of $\mathcal{H}$.

$$
\begin{aligned}
\mu_{\psi^1+\psi^2}(B) &= \|P(B)(\psi^1 + \psi^2)\|^2 \\
&= \mu_{\psi^1}(B) + \mu_{\psi^2}(B) + (P(B)\psi^1, \psi^2) + (\psi^2, P(B)\psi^1)
\end{aligned}
$$

and

$$
(P(B)\psi^1, \psi^2) = (P(B)[\mathcal{H}_1]\psi^1, [\mathcal{H}_2]\psi^2) = 0
$$

for every Borel set B if and only if the two subspaces are orthogonal and one of them, say $\mathcal{H}_1$, is H-invariant (and, hence, $[\mathcal{H}_1]$ commutes with $P(B)$ for all B). Then, however, $\mathcal{H}_2 \subset \mathcal{H}_1^\perp$ which is H-invariant and contains ψ^2.

6.2.1

Choose a sequence $\{n_k\}$ such that $V^k \equiv V(T^{n_k}\omega) \to V(\omega')$ pointwise. The corresponding operators $H^k = H_0 + V^k$ all have the same spectrum, $\sigma(H(\omega))$, and converge strongly to $H(\omega')$. Equation (6.1) holds in the form $\sigma(H(\omega)) \supset \sigma(H(\omega'))$. The opposite is also true because $V(\omega')$ is also minimal.

6.2.2

Any point in the spectrum which is not an eigenvalue is in the essential spectrum. So we have to prove that all the eigenvalues are in the essential spectrum. Let E be an eigenvalue, ψ the corresponding normalized eigenvector. Because V is recurrent, there exists an increasing sequence $\{n_k\}$ such that $V^k = T^{n_k}VT^{-n_k}$ ($V_n^k = V_{n+n_k}$) tends to V pointwise. Let $\varphi^k = T^{-n_k}\psi$. This goes to zero weakly ($(\varphi, \varphi^k) \to 0$ for any fixed vector φ), so it is a Weyl sequence if $\varepsilon^k \equiv (H_0 + V - E)\varphi^k \to 0$ (in norm!).

$$
\|\varepsilon^k\|^2 = \|T^{n_k}\varepsilon^k\|^2 = \|(H_0 + V^k - E)\psi\|^2 = \|(V^k - V)\psi\|^2
$$

There exists a sequence of integers $m_k \to \infty$ and a sequence $\eta_k \to 0$ such that $|V_n^k - V_n|^2 < \eta_k$ for $|n| < m_k$, and $\sum_{|n|\geq m_k} |\psi_n|^2 < \eta_k$. Therefore

$$
\|(V^k - V)\psi\|^2 = \left(\sum_{|n|<m_k} + \sum_{|n|\geq m_k} \right)(V_n^k - V_n)^2|\psi_n|^2 < \eta_k(1 + 4\sup|V_m|^2)
$$

so ε^k goes to zero, indeed.

6.9.1

According to Section 6.3, the IDS can be obtained as

$$
\mathcal{N}(E) = \lim_{n\to\infty} \mathcal{N}_{nL}(E)
$$

where $\mathcal{N}_{nL}(E)$ is $1/nL$ times the number of eigenvalues less than E of H_{nL}, the restriction of H to an interval of length nL. A convenient choice of boundary condition is

$$\psi(k + nL) = e^{i\alpha}\psi(k)$$

The matrix of H_{nL} has $V_1, ..., V_{nL}$ in the diagonal, 1 above and below it and $e^{-i\alpha}$ and $e^{i\alpha}$ in the upper right and lower left corner, respectively. Finding the eigenvalues of H_{nL} is equivalent to finding the E values for which the transfer matrix $T_{1\to nL}(E) = T_{1\to L}^n(E)$ has eigenvalues $e^{\pm i\alpha}$ or trace $2\cos\alpha$: this can be seen from

$$\Psi_{nL} = T_{1\to nL}\Psi_0$$

(cf. Section 3.2) and the boundary condition. Choose $\alpha = \pi/2$, then one has to look at the zeros of $\operatorname{tr} T_{1\to L}^n(E)$. From Figure 1 and Problem 3.2.1 one learns that this function has exactly n zeros in each band of the spectrum of H; therefore the IDS in the gap just above the kth band is $kn/nL = k/L$, independently of n, which proves the assertion.

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